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GC-MS (Gas Chromatographic-Mass Spectrometric) Suitability Testing of RCRA Appendix VIII and Michigan List Analytes

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As a first step in a hierarchical scheme to demonstrate the suitability of present U.S. Environmental Protection Agency (USEPA) analysis methods and/or develop new methodology, the gas chromatographic (GC) separation and mass spectrometric (MS) detection characteristics of 328 toxic and/or hazardous organic materials have been investigated. Volatile and semivolatile analytes were tested using the GC/MS conditions specified in the USEPA Methods 8240 and 8270, respectively, as modified by the Contractor Laboratory Program (CLP) protocol. Standard mixtures of analytes were analyzed by septum injection onto the analytical column without any prior sample work-up procedures.

For the 187 analytes that proved suitable for GC/MS analysis by Methods 8240 and 8270, the relevant characteristics for GC retention (retention time and relative retention index) and for MS detection (recommended quantification ion and confirmation ions with relative abundances and response factor relative to the internal standard) are reported. For analytes not detected by GC/MS or not included, a priori, recommendations for future work are made.

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GC-MS SUITABILITY TESTING OF RCRA APPENDIX VIII AND MICHIGAN LIST ANALYTES

by

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FOREWORD

Environmental measurements are required to determine the quality of ambient waters and the character of waste effluents. The Environmental Monitoring and Support Laboratory - Cincinnati, Ohio conducts research to:

- Develop and evaluate methods to measure the presence and concentration of physical, chemical, and radiological pollutants in water, wastewater, bottom sediments and solid waste.
- Investigate methods for the concentration, recovery, and identification of viruses, bacteria and other microbiological organisms in water; and, to determine the responses of aquatic organisms to water quality.
- Develop and operate an Agency-wide quality assurance program to assure standardization and quality control of systems for monitoring water and wastewater.
- Develop and operate a computerized system for instrument automation leading to improved data collection, analysis, and quality control.

This report describes an investigation as to the suitability of GC-MS methodology contained in SW-846 Methods 8240 or 8270 for organic non-priority pollutant analytes from RCRA Appendix VIII and the Michigan list.

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ABSTRACT

As a first step in a hierarchical scheme to demonstrate the suitability of present US EPA analysis methods and/or develop new methodology, the gas chromatographic (GC) separation and mass spectrometric (MS) detection characteristics of 328 toxic and/or hazardous organic materials have been investigated. The analytes in question are the organic substances in the RCRA Appendix VIII listing plus those on the "Michigan List" which have been proposed to be added to the Appendix VIII list. EPA priority pollutants were omitted from this work since they are already thoroughly characterized. Volatile and semivolatile analytes were tested using the GC-MS conditions specified in US EPA Methods 8240 and 8270, respectively, as modified by the Contractor Laboratory Program (CLP) protocol. Reference analytes were obtained primarily from EPA repositories and secondarily from commercial suppliers. Standard mixtures of analytes were analyzed by septum injection onto the analytical column without any prior sample work-up procedures (i.e., extraction of semivolatiles from water and purge-trap-desorb analysis of volatiles were omitted).

For analytes that proved suitable for GC-MS analysis by Methods 8240 and 8270, the relevant characteristics for GC retention (retention time and relative retention index) and for MS detection (recommended quantification ion and confirmation ions with relative abundances and response factor relative to the internal standard) are reported. For analytes not detected by GC-MS or not included, a priori, recommendations for future work are made.

Results for the 328 non-priority pollutant analytes considered for this work can be summarized as follows:

Number of Analytes	Category
33	Volatile analytes suitable for Method 8240 GC-MS conditions
6	Volatile analytes detected with low response factors
139	Semivolatile analytes suitable for Method 8270 GC-MS condition

9	Semivolatile analytes detected with low response factors
15	Volatile analytes not detected
45	Semivolatile analytes not detected
58	Omitted *a priori* due to obvious inapplicability of direct GC analysis
31	Not obtainable
336	
(8)	Analytes tested by both methods
328	Total number of analytes considered

Only 2 of the 8 non-detected volatile analytes which were retested as semivolatile analytes were detected using those conditions. Eleven of the 139 semivolatile analytes judged suitable for Method 8270 GC-MS conditions were so classified based on the results of other EPA studies using GC-FID. Even though these 11 analytes were not detected in the present work, they can nevertheless be recommended for inclusion in future Method 8270 testing.

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SECTION 1

INTRODUCTION

The Resource Conservation and Recovery Act (RCRA) (1) specifies over 300 toxic organic compounds in its Appendix VIII listing which may be used to identify hazardous wastes. In response to a petition by the state of Michigan, the U.S. Environmental Protection Agency (EPA) has proposed the amendment of RCRA Appendix VIII by the addition of over 100 other organic compounds to give a total of over 400 organic constituents (2). Gas chromatographic methods for determining organic compounds in wastes are given in SW-846, "Test Methods for Evaluating Solid Wastes". In many cases these methods are modifications of procedures for the determination of some, but not all, of the Appendix VIII and Michigan List compounds in wastewater. EPA is currently attempting to validate analytical methods for as many of these 400 plus compounds as possible. A hierarchical approach to these validation efforts is being pursued.

An example of a hierarchical approach to the development and validation of analytical methods for the determination of organic compounds in wastes is presented in Figure 1. The first phase of this approach defines the scope of work for the research program reported here and involves the identification of compounds which are amenable to GC separation and MS detection. These evaluations involved the analyses of solutions of standard materials using the GC-MS conditions described in the Contractor Laboratory Protocol (CLP) for the application of US EPA Methods 8240 and 8270 for volatile and semivolatile organic compounds, respectively.

This report describes the procedures and presents the results obtained from implementation of this first phase of the hierarchical approach. The compounds were classified as candidates for Method 8240 or Method 8270 testing. Some compounds were not tested because they fell into one of the following categories:

- Priority pollutants -- The chromatographic behavior of these compounds has already been thoroughly characterized.
- Unstable -- Compounds known to degrade rapidly in aqueous sample matrices.

- Not amenable to gas chromatography -- Compounds known to be too polar and/or too thermolabile to elute using Method 8240 or Method 8270 conditions.
- Not avaliable -- Compounds for which standards were not available either from the EPA repository or from commercial sources.

For compounds determined to be amenable to these methods, the following data were obtained:

- GC Performance -- retention characteristics.
- Mass Spectral Performance -- response factors, key ions for detection and quantification using extracted ion current profiles (EICP).

Figure 1 is presented to show the context in which the work reported here will lead to subsequent method development activities. For example, compounds which are not amenable to determination by GC-MS are to be evaluated in future programs for the feasibility of alternate approaches including special GC conditions, derivatization prior to GC analysis, high performance liquid chromatography (HPLC), and/or non-chromatographic methods. Compounds which are amenable to GC-MS in the work reported here are to be subjected to further method performance evaluation. Volatile compounds will be evaluated for amenability to the purge-trap-desorb (PTD) techniques described in Method 5030.

For compounds which are not successfully recovered from an aqueous matrix using this procedure, alternate procedures such as heated PTD, direct liquid injection (DLI), or the Method 5020 headspace sample introduction technique can then be evaluated. Compounds which are successfully recovered using the Method 5030 room temperature PTD procedure can be included in a validation study of Methods 5030/8240 using the procedures described in the Single Laboratory Method Validation Protocol which was developed during an earlier Work Assignment of this contract.

The semivolatile compounds shown to be amenable to GC-MS determination will be evaluated for amenability to the extraction procedures described in Method 8270. For compounds which are not successfully recovered

from an aqueous matrix using this procedure, alternate extraction schemes and novel techniques, such as solid phase extraction (SPE), can be considered. Compounds successfully recovered using the Method 8270 extraction procedure can be included in evaluations of several sample cleanup procedures. These investigations will involve fortifying a wide variety of waste matrices with the compounds to permit selection of appropriate cleanup procedures for compounds/sample matrix combinations. Ultimately, these compounds will be included in a validation of Method 8270 in conjunction with various cleanup techniques using the Single Laboratory Method Validation Protocol.

Implementation of the hierarchical method development approach is expected to result in the development of a suite of analytical methods consisting of a limited number of procedures for the determination of a large proportion of the more than 400 organic compounds. This limited number of analytical procedures for extraction steps, cleanup steps, and determinative steps will form the core of a generic approach to the selection of appropriate analytical methods addressing hazardous wastes. The system will be generic in the sense that the specifications of type of analyte, type of matrix, and type of sensitivity and required specificity will generate, from the limited suite of component analytical procedures, the most appropriate set of analysis conditions.

The reduction in the number and variety of methods required to characterize wastes that this type of generic approach will allow will provide cost benefits both to the government and to the regulated community. This generic approach will facilitate periodic updates as new information becomes available about specific analytes in specific matrices. Another advantage of this generic approach is that the areas requiring method modification or method development will be clearly identified. Consequently, this collection of research requirements can then be prioritized for resource allocation.

SECTION 2

CONCLUSIONS

After the elimination of redundancies, the Appendix VIII and Michigan list compounds include 440 organic compounds. The classification of these compounds and results of testing them for suitability for inclusion in present volatile and semivolatile analysis methods are summarized as follows:

Analytes Considered				
Tested for GC-MS Suitability				239*
Omitted Priority Pollutant				112
Omitted A Priori				58
Not obtainable				31
Total Considered				440
Volatile Analyte Testing				
Suitably Detected	33			
Detected with Low Response Factor		6		
Not Detected		15		
Sub Total	33	+ 21	=	54*
Semivolatile Analyte Testing				
Suitably Detected	128			
Expected to be Suitable	11			
Detected with Low Response Factor		9		
Not Detected		45		
Sub Total	139	+ 54	=	193*
Total Suitable	172			
Total Not Suitable		75		
Total Tested				247*

*Eight of the analytes that failed volatile testing were carried into the semivolatile testing. Two of these eight analytes were suitably detected in semivolatile testing.

One-hundred twelve priority pollutants were eliminated from testing because they have already been fully characterized by these methods; 58

compounds were eliminated a priori because they are known to be unstable in water or unsuitable for determination using Method 8240 or 8270 conditions; and 31 compounds were eliminated because a source of the analyte could not be identified. Chloral, also eliminated because of its unavailability, was replaced by the compound which it forms immediately on contact with water, chloral hydrate. Therefore, a total of 239 compounds was included in these evaluations.

Six of the 39 volatile analytes detected by GC-MS were found to have unacceptably low response factors (less than 0.02) relative to benzene-D6. Similarly, 9 of the semivolatile analytes detected were found to have unacceptably low response factors relative to phenanthrene-D10. For 11 of the semivolatile analytes not detected in this study, other information such as GC-MS and/or GC-FID results on other research programs indicates that these analytes should be suitable for GC-MS analysis and therefore have been included in the tabulated results. Reasons that 15 of the volatile and 45 of the semivolatile analytes were not detected might include one or more of the following:

- Thermolability -- The thermolability of these analytes might be less than anticipated and the analytes degraded in the GC injector or on the column.
- High polarity -- Some of these analytes might be more polar than anticipated and they either did not elute from the column in a reasonable length of time or their chromatographic behavior was so poor that they eluted from the column over a long period of time.
- The reference standard used may not have been the analyte it was identified to be. The compound may have degraded in the solvent in which the stock or injection standard was prepared or may have reacted with another analyte present in the same mixture.

Compounds omitted or those for which GC-MS analysis was found to be unsuitable were further classified according to future method development requirements in the heirarchical scheme. The categories into which the non-suitable analytes were grouped were:

- Direct HPLC-MS (66 compounds)
- Derivitization followed by GC (10 compounds)
- Derivitization followed by LC (6 compounds)
- Further direct GC investigation (i.e., the non-suitability results were anomalous, (12 compounds)
- No recommendations can be made at this time (11 compounds).

For the 39 volatile and 137 semivolatile compounds which were detected by GC-MS analysis key GC performance and mass spectral data were obtained. These data are presented in this report.

SECTION 3

RECOMMENDATIONS

The general recommendation arising from the data and results generated in the studies presented in this report is to continue implementation of the hierarchical research strategy. The following specific recommendations are made:

- The 39 volatile compounds detected using the GC conditions of Method 8240 should be included in an evaluation of the Method 5030 PTD sample introduction.
- Extractability studies of the 137 semivolatile compounds detected using the GC conditions of Method 8270 conditions should be conducted.
- The 11 compounds which were anomalously not detected should receive more detailed examination.
- Compounds which were not found to be amenable to GC-MS analysis should to be tested in the alternate methodologies specifically recommended for them.

SECTION 4

EXPERIMENTAL

ANALYTE CLASSIFICATION

The initial set of analytes consisted of organic compounds included in RCRA Appendix VIII (Federal Register, October 1, 1984) plus those included in the Michigan petition (Federal Register, December, 1984) minus the EPA priority pollutants. After eliminating redundancies in the two lists, remaining compounds were classified as to their predicted suitability for SW 846 Method 8240 (volatiles), Method 8270 (semi-volatiles), or for their predicted inability to be determined by either method.

ANALYTE PROCUREMENT

Sources for the selected analytes were identified in the following order of priority: 1) the EPA repositories of reference compounds and pesticides (EMSL - Las Vegas and RTP), 2) the EPA repository of certified solutions (EMSL - Cincinnati), and 3) commercial suppliers. A list of synonyms for each compound was generated using CAS/on-line so that all commercial suppliers listed in the 1985 edition of Chem Sources would be identified. When multiple sources for compounds were available, the priority of commercial vendors was approximately: Aldrich, Fluka, Pfaltz & Bower, Eastman, Sigma, and Chem Services. Other sources were used if these companies could not supply the compound. Neat analytes were stored at ambient temperature or at -10°C when refrigeration was recommended by the supplier. The sources and supplier-claimed purities are shown in Table 1 for volatile analytes and Table 2 for semivolatile analytes.

STOCK SOLUTIONS

Stock solutions of individual analytes were prepared at 1% (w/v) unless low solubility required greater dilution. Solutions from neat samples were prepared by weighing the solid or liquid into either a tared glass container or an aluminum foil square, after which the analyte was diluted with

solvent to produce a 1 percent concentration. Generally, approximately 40 mg (weighed to the nearest 0.1 mg using an analytical balance) was diluted with the correct volume of solvent measured with a 5-mL syringe. The approximate 4 mL of solution was stored in a 4.5 mL glass vial with a Teflon-lined screwcap lid. Analytes which required additional dilution were rinsed into a larger vial with similarly measured diluent.

For the two gaseous analytes, ethylene oxide and methyl mercaptan, the gas was bubbled into a 50 mL volumetric flask partially filled with solvent and placed on a top loading balance. Gaseous flow continued until the weight of gas was approximately 0.50 grams. After weighing on an analytical balance, additional solvent was added to yield a 1.0 percent (w/v) solution. Stock solutions were usually prepared no more than two weeks in advance of analysis and were stored at -10 C.

Volatile analyte stock solutions were prepared in methanol. Methylene chloride was used for most of the semivolatiles; however, some required methanol, acetone, or benzene as co-solvents or alternative solvents to dissolve the analyte. When dictated by solubility considerations, less concentrated stock solutions were prepared (i.e., 0.5 to 0.1 percent).

Four compounds, auramine, 3-(chloromethyl)pyridine, 2,4,-diaminoanisole, and phenazopyridine, were received as acid salts. These compounds were converted to their free bases by reaction with aqueous K_2CO_3 followed by extraction with methyl tert-butyl ether (MTBE). These free bases were used as recovered in MTBE solution in amounts based on residue weight analysis and the assumption that the recovered material was the pure free base.

INJECTION STANDARDS

GC-MS suitability studies were performed using analyte mixtures prepared after consideration of chemical reactivity. Because mass spectral detection was employed, compound coelution was not a major factor unless isomeric analytes were being considered for the same mixture. Volatile and semivolatile mixtures of stock solutions were diluted to the correct concentration for GC-MS analysis using methanol or methylene chloride, respectivley. All injection standards were analyzed on either the day of preparation or the following day.

Individual analyte concentrations in the volatile mixtures were 200 ug/mL for most of the analytes or 400 ug/mL for a few analytes predicted to exhibit lower response factors. Concentrations as high as 2000 mg/mL were prepared for the repeat analysis of some volatile analytes not detected in the first attempt. Thus, the 1.5 uL injections of volatile analytes provided a minimum of 300 ng of analyte on column. The concentrations of individual semivolatile analytes in the injection standards were usually 40 ug/mL. For analytes not detected on the first attempt, higher concentrations were employed, ranging from 50-400 ug/mL. Thus, the 2 uL injections of semivolatile analytes provided a minimum of 80 ug of analyte to the splitless injection evaporator cavity.

Internal standards specified in the CLP for both volatile and semivolatile analyses were used to provide measures for both relative retention index (RRI) and response factor (RF). Surrogate standards specified in the CLP were included in volatile analyte mixtures but not for the semivolatile mixtures since the significantly greater number of them in the latter case would have made the data interpretation somewhat more difficult without any benefit to the usefulness of the results obtained.

Table 3 lists the composition, purity, and stock solution concentration for the internal standards used in volatile and semivolatile analyses. Bromofluorobenzene (BFB) and decafluorotriphenylphosphine (DFTPP) were also added to each mixture as mass spectrometric tuning standards to enable verification that the MS ion source tuning conditions were within acceptable limits for each chromatographic analysis.

INSTRUMENTATION

Balances

In most cases, analytical balances readable to 0.01 or 0.1 mg (Mettler Models HL-32 and HL-52, respectively) were used to weigh neat analytes. Analytes in extremely short supply were weighed on a microbalance readable to 0.001 mg (Mettler ME-30).

GC-MS Systems

A Finnigan 3200 MS with Finnigan 9500 GC and a glass-jet separator GC to MS interface was used for volatile analytes. Two instruments were used for semivolatile analytes: A Finnigan 3200 MS with a Carlo Erba 4160 GC and a Finnigan 5100 GC-MS system with a Finnigan Model 9610 GC. All three MS instruments were equipped with a -3kV conversion dynode ahead of the continuous-stage electron multiplier. Both instruments used for semivolatile analyses had GC to MS transfer section designs which enabled placing the fused silica column outlet just inside the MS ion source cavity. A Finnigan INCOS data system with software revision 3.1C and the 1983 EPA/NIH MS library of 39,763 spectra was used for all data processing.

ANALYSIS CONDITIONS

The CLP GC and MS analysis conditions, shown in Table 4, were used in all cases. For the volatile analytes, the solvent diverter was not used and data collection was not interrupted during the methanol solvent elution.

Each day that volatile or semivolatile analyses were performed, the ion source tuning was adjusted to give the correct spectrum for BFB (volatile analyte analysis) or DFTPP (semivolatile analysis). The BFB was introduced by batch mode while the DFTPP was introduced through the GC. The ion mass-detection sensitivity criteria, as specified in the CLP, are shown in Table 5. For the volatile analyte work, the BFB criterion for m/e 176 (between 95 and 100 percent of m/e 174) was often not achievable; typically it was between 93.5 and 94.9 percent of m/e 174. In those cases, data acquisition proceeded since the deviation did not have any practical consequence on the mass spectra or response factors generated. Otherwise, the BFB and DFTPP criteria were met before proceeding with data acquisition.

GC-MS DATA PROCESSING

Initially, a list of the analytes that were represented in the mass spectral library base was created using a CAS number-based computer-operated search of the EPA/NIH mass spectral library. These abbreviated library reference mass spectra were then printed for later use in confirming peak identities or for searching data files. The GC-MS data processing activities which were performed on each GC-MS data file were as follows:

1. Queue the mass spectra of the detected GC peaks for automated spectral matching against the library.
2. Print expanded chromatograms and the automated mass spectral library matching results together with the uncorrected and background-subtracted mass spectrum for each GC peak.
3. Inspect the library matching output and label GC peaks in the expanded chromatogram according to their identification.
4. Reverse search the data files for analytes known to be in the analyzed mixture but not identified in Step 3.
5. Tabulate the analysis results: Scan number of the GC peak, recommended quantification ion, recommended confirmation ions and their abundances.
6. Review of the results of Steps 3, 4, and 5 by a senior mass spectroscopist with further data processing as deemed necessary to document the quality of the identification results and/or the non-detection of analytes.
7. Integrate and tabulate EICP's of quantification ions for the validated analyte identifications.

PERSONAL COMPUTER DATA MANAGEMENT

Initial analyte classifications and the information generated in the GC-MS data processing were transferred to a personal computer, PC, for management using Lotus/Symphony software. The information transferred to the computer for each analyte included:

- Name
- Designation of whether the compound was from Appendix VIII or the Michigan list
- Designation of initial analyte classification (i.e., volatile, semivolatile or omitted)
- CAS number
- RCRA number
- MS library entry number
- Commercial source (including EPA) and purity or designation if not commercially available.

For analytes that were identified in the GC-MS data, additional information entered included:

- The scan number of the GC peak
- The recommended quantification ion
- The recommended confirmation ions and their abundances
- The response factor for MS detection versus the internal standard.

The PC was used to compute GC retention times, relative GC retention indices and to sort and compile separate listings by categories related to the status of information about the analytes.

SECTION 5

RESULTS AND DISCUSSION

SELECTION AND PROCUREMENT OF ANALYTES TO BE TESTED

After elimination of redundancies, the combined Appendix VIII and Michigan analyte sets contain 440 compounds, 112 of which are already thoroughly characterized EPA priority pollutants. Thus, 328 substances qualified for the present scope of work. Each was classified according to whether it was expected to be amenable to analysis by Method 8240 (volatile analytes) Method 8270 (semivolatile analytes) or neither method. The results of this classification are shown in Table 6.

Eight of the compounds in Table 6 are classified both as volatile and semivolatile since, after failing to elute in the volatile compound testing, they were carried into the semivolatile compound testing. The 58 compounds indicated in Table 6 as being omitted a priori are separately listed in Table 7 with the specific reason for omission and a recommendation for future method development work. These reasons for a priori omission and suggestions for future method development can be classified as follows:

- Acids - 14 Compounds. Typically, these acids are carboxylic acids or are of comparable strength and require derivatization to achieve acceptable GC performance.
- Nonvolatile - 12 compounds. These analytes are so polar and/or of such high molecular weight that there is essentially no possibility of their elution from a GC column. Typical of these compounds are macrolytic antibiotics and dye molecules for which HPLC rather than a derivatization-GC approach is appropriate for most cases.
- Hydrolytically or otherwise unstable - 9 compounds. Since groundwater and wet soils and sludges are sample matrices of interest, there is no need to demonstrate analysis capability for compounds which decompose rapidly in these sample types.

- Aldehydes - 6 compounds. Special GC conditions have been used successfully for a number of these analytes but, generally, the associated sample work-up procedures are not fully successful in preserving these reactive analytes prior to their detection. Therefore, derivatization followed by HPLC with UV detection which has been shown to be sensitive and reproducible for formaldehyde, is clearly the favored analytical approach for these compounds. Thus, there was no need to include them in GC method testing.
- Redundancies - 5 compounds. These compounds typically are salts of a free base also listed as an analyte. Diphenylamine was considered redundant with the priority pollutant, N-nitrosediphenylamine since the latter is known to decompose quantitatively to the former in GC injectors.
- Inappropriate for inclusion in the present scope for miscellaneous reasons - 12 substances. Some analytes were considered inappropriate because they can hardly be considered organic analytes. Examples of this category include hydrazine, thiosemicarbizide, semicarbizide, thiourea and dithiobiuret. Others are currently, or are expected to be, appropriately addressed by other specialized methods. Examples of this category include TCDD and polychlorinated and polybrominated biphenyls. Two substances, coal tars and creosote, are far too heterogeneous for inclusion in Method 8270. Epinephrine had to be omitted since it could not be dissolved at sufficiently high concentration in any reasonable GC injection solvent. See Table 7 for recommendations for each of these 12 analytes.

Following elimination of the analytes listed in Table 7, sources were sought for the remaining 269 analytes. The sources and purities of the analytes obtained in time to be included in this study are presented in Tables 1 and 2. The 32 analytes that could not be obtained in time to be included in this work are listed in Table 8. One of these, chloral, is available as the hydrate which was included in the volatile analyte testing. Thus, the summary

listings show 31 analytes as "unavailable". With only a few exceptions, the Table 8 compounds were not listed as available from any supplier in the 1985 edition of Chem Sources.

RESULTS OF VOLATILE ANALYTE TESTING

The 54 volatile analytes tested with the Method 8240 GC column, 1 percent SP1000 on Carbopack B, are listed in Table 9 in which the status is indicated as satisfactorily detected (S), detected with a response factor below 0.02 (LR), or not detected (ND). The 39 compounds with status S or LR are repeated in Table 10 with their respective GC retention time, GC retention index relative to benzene-D_6, key ions and relative abundances to be used for detection and quantification, and response factor relative to benzene-D_6. The six compounds with response factors lower than 0.02 are bis-(2-chloroethyl) sulfide, chloral hydrate, 2-chloroethanol, 2-hydroxypropionitrile, propargyalcohol, and n-propylamine. Although the very low response factors can be expected to result in unacceptably high MDL values for Method 8240, their relevant GC and MS data are included for reference information.

Table 11 lists the 15 volatile analytes that were not detected using the Method 8240 conditions and gives recommendations for future method development work. All of these non-detected analytes were analyzed at least twice, with the repeat analysis usually at 2 to 5-fold higher levels than the original 300 ng level. Three of those 15 analytes, hexachloropropene, tetranitromethane, and thiophenol were thought to have failed to elute due to boiling points and/or polarities that were too high for the SP1000/Carbopack B column, and these compounds were retested using the Method 8270 (semivolatile analyte) conditions.

Non-detection of the hydrazines and aziridines (6 analytes) was probably due to extreme GC peak tailing on the SP1000/Carbopack B column, even though all of the amines were analyzed at the very high level of 1000 ng/uL (note, for example, the very low 0.002 response factor shown for butylamine in Table 11). Five of these nitrogen bases were also tested with the semivolatile analytes. The sixth, N(2-hydroxyethyl)ethyleneimine, was not tested due to its extreme polarity.

2-Butanone peroxide apparently quantitatively decomposed to 2-butanone in the injector. Methyl mercaptan apparently coelutes with methanol

on the SP1000/Carbopack B column and, in this case, would be substantially lost at the jet separator due to the presence of the methanol vapor displacement of the helium carrier. The remaining 4 un-detected volatile compounds were not repeated in the semivolatile set since they were too volatile to be recovered in a KD distillation of extraction solvent. All 4 of the non-detected analytes (2 haloethers, methyl isocyanate and 2-methyllactonitrile) are known to be chemically labile, and, therefore, were not pursued further.

RESULTS OF SEMIVOLATILE ANALYTE TESTING

The 185 semivolatile analytes plus the 8 retested volatile analytes which were also analyzed with the Method 8270 GC column, fused silica capillary with methylphenyl silicone phase, are listed in Table 12. The status is indicated as satisfactorily detected (S), expected to be satisfactory for GC-MS determination based on other information (ES), detected with a response factor less than 0.02 versus phenanthrene-D_{10} (LR), or not detected (ND).

Table 13 lists the 137 analytes detected with satisfactory or low response factors and provides the same kind of results as tabulated for the volatile analytes in Table 10. The analytes detected with low response factors are 1-acetyl-2-thiourea, barban, 2-cyclohexyl-4,6-dinitrophenol, diethyl sulfate, 3,3'-dimethoxybenzidine, 4,4-methylenebis(2-chloroaniline), octamethyl pyrophosphoramide, propylthiouracil, and tris(2,3-dibromopropyl) phosphate. All 9 of these analytes are highly polar and reasonably expected to be sensitive to thermal decomposition in the injection.

Four compounds included in Table 13, demeton, diethylstilbesterol, tricresyl phosphate, and diallate, produced multiple GC peaks. For demeton, results from other research programs showed that demeton-O eluted before demeton-S under the same chromatographic conditions. Using that GC result and the supplier's specification that the isomer ratio was 54 percent demeton-O and 39 percent demeton-S, the isomer assignments and response factors could be calculated.

In the case of diethylstilbesterol (DES), the GC-MS data clearly indicate that the 300C GC injection condition resulted in the partial conversion of trans DES to 20 to 40 percent cis isomer and that during chromatography either part of the cis isomer produced reconverted to trans and/or part of the trans isomer remaining converted to the cis isomer. It is

known that the cis isomer slowly reverts to the trans form, which is the only isomer form in which DES is supplied. This cis isomer pre-eluted the trans by about 35 seconds (as would be predicted based on molecular geometry), eluting at about 260C, with additional DES detected in a plateau between the two isomers, demonstrating the on-column isomer interconversion. The Table 13 GC results are for the major, trans DES isomer. Since the major features of the mass spectra from the cis and trans isomers are identical, the quantification ion and search ions could be recommended with confidence, and the response factor is based on the sum of both isomers.

For tricresyl phosphate, the original sample obtained from Chem Service was apparently a technical grade containing a plethora of isomers including some that are partially or fully phosphate esters of C_2-phenols instead of methyl phenols. The work was repeated with a bona fide sample of tris(p-tolyl) phosphate which gave a single GC peak, and the GC retention and MS detection parameters of Table 13 are for the single isomer. The range of GC retention for technical grade cresyl phosphate is given in Table 13 as a footnote.

Diallate was present, as supplied, as both the cis and trans isomers, which apparently do not interconvert during chromatography and were clearly separated. However, no information about the elution order of the isomers is available, thus isomeric identification of the two peaks is not possible. The response factor given is for the sum of the two peaks.

Table 12 contains 11 analytes that are indicated with status "ES", which designates that non-detection of the analyte is considered anomalous. These 11 analytes are listed separately in Table 14. All 11 of these analytes were found to be suitably analyzed in Work Assignment 2-08 of this contract in which analytes were extracted from spiked aqueous standards, concentrated and analyzed by fused silica capillary GC-FID. Thus, although MS data was not obtained in the WA 2-08 work, it seems reasonable to classify their non-detection in the present work as anomalous.

A second analysis at 5-fold higher level, 400 ng into the GC injector cavity, was performed for 5 of the Table 14 analytes (4-chloro-1,2-phenylenediamine, diazinon, 4,4'-methylenbis (N,N-dimethylaniline), 2-naphthylamine, and tetraethyldithiopyrophosphate), and a second analysis was performed for 3-amino-9-ethylcarbazole at 2.5-fold higher level (200 ng injected). The other 5 analytes were only analyzed once. Except for the two

organophosphates, the anomalously non-detected Table 14 analytes are strongly basic molecules, so that a possible explanation for their non-detection would be that the column used was somewhat acidic.

The 45 analytes for which non-detection in the GC-MS data cannot be classified as anomalous are listed in Table 15. Generally, these analytes are highly polar or are labile to decomposition before or during chromatography. Comments regarding a probable or possible cause for non-detection in this work and suggestions for future method development are also presented in Table 15. Four of the 45 analytes are aromatic diamines, 1,2-and 1,3-phenylenediamine, 2,4-diaminoanisole, and 1,5-naphthalendiamine. These 4 analytes can probably be analyzed by fused silica GC if special precautions are taken to ensure good performance for basic materials. Ethylene thiourea (ETU) has been shown in previous work in our laboratory to be amenable to GC analysis using special conditions (see Footnote (f) in Table 15). For another six analytes, polarity, volatility and lability considerations apparently do not account for the non-detection, and, therefore, a more thorough attempt to develop GC-based methods might be successful (see Footnote (d) in Table 15).

For the remaining 34 analytes, the causes of non-detection can be speculated as follows:

18 analytes:	exceptionally high polarity
9 analytes:	thermal or chemical lability
4 analytes:	both of the above
3 analytes:	not volatile enough, principally due to molecular weight or geometry rather than polarity

Recommendations for further method development for the 34 Table 15 analytes for which non-GC methods seem to be required are classified as follows:

30 analytes:	HPLC, including ion chromatography, method development recommended
2 analytes:	HPLC-post column derivitization method has already been demonstrated
2 analytes:	no method development approach is recommended at this time

One of the analytes recommended for HPLC method development (trichlorfon) has been shown in previous work to be extremely labile to aqueous conditions and splitless, evaporator cavity GC injection. For non-aqueous samples and sample work-up procedures, cold, on-column GC has been shown to be a feasible but troublesome solution for trichlorfon.

REFERENCES

1. 40 Code of Federal Regulation, Part 261.
2. Federal Register, 49, No. 247, December 21, 1984, pp. 49784-49793.

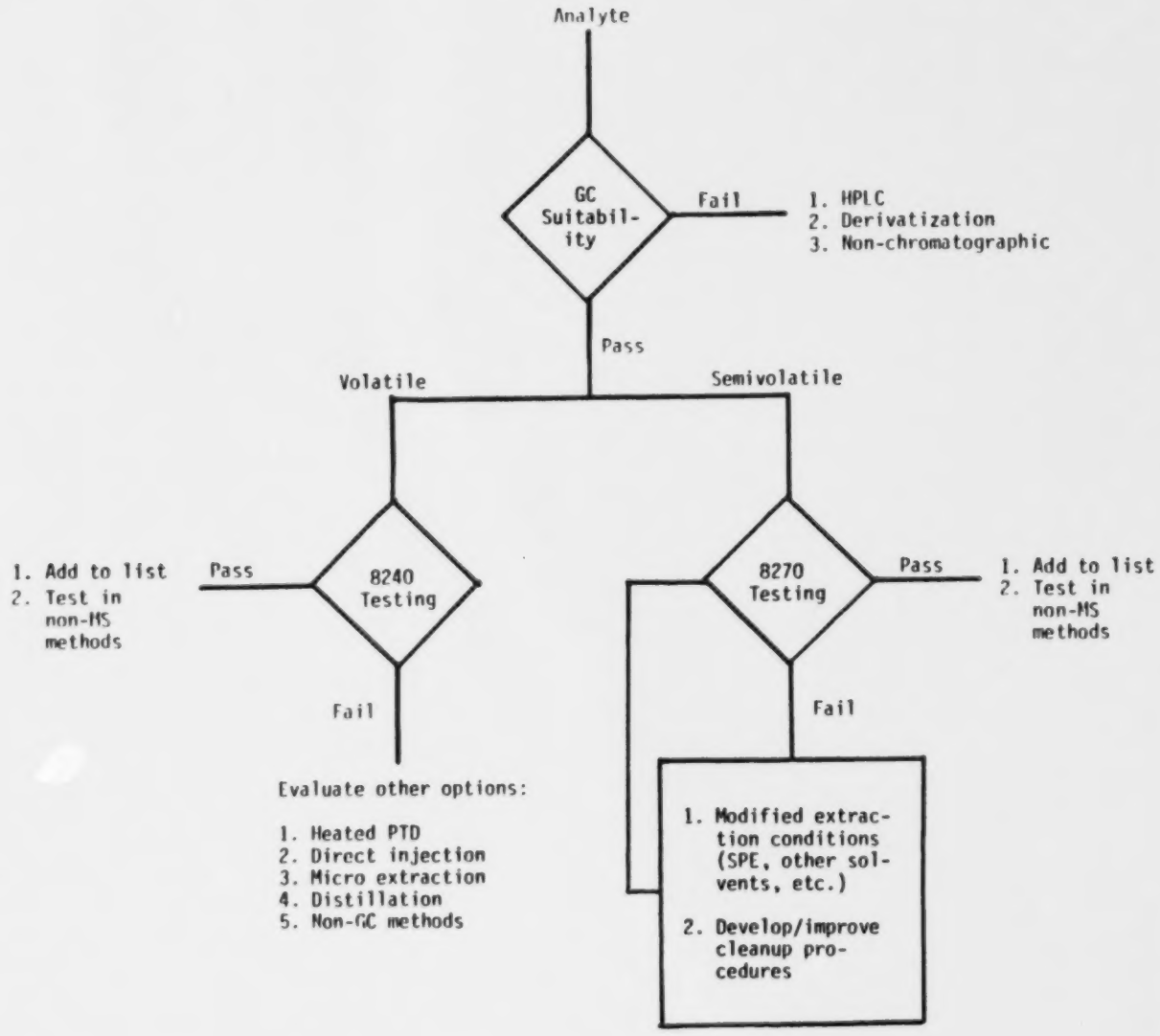

Figure 1. Heirarchical Approach for Analytical Method Development for Organic RCRA Analytes.

TABLE 1. SOURCES AND PURITIES OF VOLATILE COMPOUNDS

INDEX	SUBSTANCE	CAS NO.	SUPPLIER(a)	% PURITY(b)
1	ACETONITRILE	75-05-8	B & J	99
2	ALLYL ALCOHOL	107-18-6	ALDRICH	99
3	ALLYL CHLORIDE	107-05-1	EPA/N	99
4	BENZYL CHLORIDE	100-44-7	EPA/N	99
5	BIS-(2-CHLOROETHYL) SULFIDE	505-60-2	BCL	NA
6	BIS-(CHLOROMETHYL) ETHER	542-88-1	CHEM SERVICE	NA
7	BROMOACETONE	598-31-2	CHEM SERVICE	NA
8	2-BUTANONE PEROXIDE	1338-23-4	ALDRICH	50 (c)
9	2-BUTANONE	78-93-3	EPA/S	NA
10	CARBON DISULFIDE	75-15-0	EPA/S	NA
11	CHLORAL HYDRATE	75-87-6	FISHER	USP
12	2-CHLOROETHANOL	107-07-3	EASTMAN	NA
13	CHLOROMETHYL METHYL ETHER	107-30-2	CHEM SERVICE	NA
14	CHLOROPRENE	126-99-8	ALFA	50 (d)
15	3-CHLOROPROPIONITRILE	542-76-7	FLUKA	97
16	1,2-DIBROMO-3-CHLOROPROPANE	96-12-8	EPA/N	98
17	DIBROMOMETHANE	74-95-3	ALDRICH	99
18	DICHLORODIFLUOROMETHANE	75-71-8	EPA/S	NA
19	1,4-DICHLORO-2-BUTENE	764-41-0	ALDRICH	85
20	1,3-DICHLORO-2-PROPANOL	96-23-1	ALDRICH	95
21	1,2,3,4-DIEPOXYBUTANE	1464-53-5	ALDRICH	97
22	1,1-DIMETHYLHYDRAZINE	57-14-7	CHEM SERVICE	95
23	1,2-DIMETHYLHYDRAZINE	540-73-8	ALDRICH	99
24	1,4-DIOXANE	123-91-1	EPA/N	99
25	EPICHLOROHYDRIN	106-89-8	EPA/S	NA
26	ETHYLENE DIBROMIDE	106-93-4	EPA/N	99
27	ETHYLENE OXIDE	75-21-8	MATHESON GAS	NA
28	ETHYLENIMINE	151-56-4	CHEM SERVICE	NA
29	ETHYL METHACRYLATE	97-63-2	ALDRICH	99
30	HEXACHLOROPROPENE	1888-71-7	ALDRICH	96
31	N-(2-HYDROXYETHYL)ETHYLENEIMINE	1072-52-2	ICN K&K	NA
32	2-HYDROXYPROPIONITRILE	78-97-7	FLUKA	85
33	ISOBUTYL ALCOHOL	78-83-1	ALDRICH	99
34	MALONONITRILE	109-77-3	ALDRICH	99
35	METHACRYLONITRILE	126-98-7	ALDRICH	99
36	2-METHYLAZIRIDINE	75-55-8	FLUKA	98
37	METHYLHYDRAZINE	60-34-4	ALDRICH	98
38	METHYL IODIDE	74-88-4	ALDRICH	99
39	METHYL ISOCYANATE	624-83-9	ALDRICH	NA
40	2-METHYLLACTONITRILE	75-86-5	ALDRICH	99
41	METHYL MERCAPTAN	74-93-1	MATHESON GAS	NA
42	METHYL METHACRYLATE	80-62-6	EPA/N	99
43	PENTACHLOROETHANE	76-01-7	EKO	NA
44	2-PICOLINE	109-06-8	EPA/N	99
45	PROPARGYL ALCOHOL	107-19-7	ALDRICH	97
46	b-PROPIOLACTONE	57-57-8	ALDRICH	99
47	PROPIONITRILE	107-12-0	ALDRICH	99
48	n-PROPYLAMINE	107-10-8	ALDRICH	98
49	PYRIDINE	110-86-1	EPA/S	NA
50	STYRENE	100-42-5	EPA/N	99

TABLE 1. (Continued)

INDEX	SUBSTANCE	CAS NO.	SUPPLIER(a)	% PURITY(b)
51	1,1,1,2-TETRACHLOROETHANE	630-20-6	EPA/N	98
52	TETRANITROMETHANE	509-14-8	CHEM SERVICE	NA
53	THIOPHENOL	108-98-5	ALDRICH	97
54	1,2,3-TRICHLOROPROPANE	96-18-4	ALDRICH	99

(a) B & J = Burdick and Jackson
BCL = Battelle in house, original supplier unknown
EPA/N = EPA neat standard
EPA/S = EPA standard solution
EKO = Eastman Organics

VSOURCE

(b) NA = Manufacturer did not supply purity.

(c) 50% 2-Butanone peroxide in dimethyl phthalate.

(d) 50% Chloroprene in xylene.

TABLE 2. SOURCES AND PURITIES OF SEMIVOLATILE COMPOUNDS

NO.	SUBSTANCE	CAS NO.	SUPPLIER(a)	PURITY(b)
1	ACETOPHENONE	98-86-2	EPA/N	99
2	2-ACETYLAMINOFLUORENE	53-96-3	P & B	NA
3	1-ACETYL-2-THIOUREA	591-08-2	ALDRICH	99
4	ACRYLAMIDE	79-06-1	EPA/S	NA
5	ALDICARB	116-06-3	EPA/N	99
6	2-AMINOANTHRAQUINONE	117-79-3	FLUKA	87
7	AMINOAZOBENZENE	60-09-3	ALDRICH	98
8	4-AMINOBIPHENYL	92-67-1	ALDRICH	99
9	3-AMINO-9-ETHYLCARBAZOLE	132-32-1	ALDRICH	90
10	AMITROLE	61-82-5	EPA/N	99
11	ANILAZINE	101-05-3	EPA/N	100
12	ANILINE	62-53-3	EPA/S	NA
13	o-ANISIDINE	90-04-0	ALDRICH	99
14	ARAMITE	140-57-8	EPA/N	96
15	AURAMINE	492-80-8	FLUKA	NA
16	AZINPHOS-METHYL	86-50-0	EPA/N	99
17	BARBAN	101-27-9	EPA/N	98
18	BENOMYL	17804-35-2	EPA/N	98
19	p-BENZOQUINONE	106-51-4	FLUKA	99
20	BROMOXYNIL	1689-84-5	EPA/N	100
21	BRUCINE	357-57-3	FLUKA	97
22	CAPTAFOL	2425-06-1	EPA/N	100
23	CAPTAN	133-06-2	EPA/N	99
24	CARBARYL	63-25-2	EPA/N	100
25	CARBOFURAN	1563-66-2	EPA/N	100
26	CARBOPHENOTHION	786-19-6	EPA/N	100
27	CHLORFENVINPHOS	470-90-6	EPA/N	95
28	4-CHLOROANILINE	106-47-8	EPA/N	99
29	CHLOROBENZILATE	510-15-6	EPA/N	99
30	5-CHLORO-2-METHYLANILINE	95-79-4	ALDRICH	97
31	3-(CHLOROMETHYL)PYRIDINE HYDROCHLORIDE	6959-48-4	ALDRICH	96
32	4-CHLORO-1,2-PHENYLENEDIAMINE	95-83-0	ALDRICH	96
33	4-CHLORO-1,3-PHENYLENEDIAMINE	5131-60-2	P & B	97
34	COUMAPHOS	56-72-4	EPA/N	97
35	p-CRESIDINE	120-71-8	ALDRICH	99
36	CROTOXYPHOS	7700-17-6	EPA/N	98
37	CUPFERRON	135-20-6	ALDRICH	ACS REAGENT
38	CYCLOHEXIMIDE	66-81-9	EPA/N	99
39	2-CYCLOHEXYL-4,6-DINITROPHENOL	131-89-5	EPA/C	NA
40	CYCLOPHOSPHAMIDE	50-18-0	SIGMA	NA
41	DEMETON (MIXED ISOMERS)	8065-48-3	EPA/N	54/39 (c)
42	DIALLATE	2303-16-4	EPA/N	50/50 (d)
43	2,4-DIAMINOANISOLE SULFATE	39156-41-7	ALDRICH	NA
44	2,4-DIAMINOTOLUENE	95-80-7	ALDRICH	98
45	DIAZINON	333-41-5	EPA/N	88
46	1,2:7,8-DIBENZACRIDINE	224-42-0	SIGMA	PRACTICAL
47	1,2:4,5-DIBENZOPYRENE	192-65-4	BCR	NA
48	DICHLONE	117-80-6	EPA/N	99
49	2,6-DICHLOROPHENOL	87-65-0	EPA/N	99
50	DICHLOROVOS	62-73-7	EPA/N	99

TABLE 2. (Continued)

NO.	SUBSTANCE	CAS NO.	SUPPLIER(a)	PURITY(b)
51	DICROTOPHOS	141-66-2	EPA/N	98
52	DIETHYLSTILBESTROL	56-53-1	GEN. BIOCHEM	NA
53	DIETHYL SULFATE	64-67-5	ALDRICH	98
54	DIHYDROSAFROLE	56312-13-1	SABER LABS	NA
55	DIMETHOATE	60-51-5	EPA/N	99
56	3,3-DIMETHOXYBENZIDINE	119-90-4	EASTMAN	TECH
57	1,4-DIMETHYLAMINOAZOBENZENE	60-11-7	FLUKA	NA
58	7,12-DIMETHYLBENZ(A)ANTHRACENE	57-97-6	SIGMA	95
59	3,3-DIMETHYLBENZIDINE	119-93-7	FLUKA	98
60	a,a-DIMETHYLPHENETHYLAMINE	122-09-8	EPA/C	NA
61	1,2-DINITROBENZENE	99-65-0	EASTMAN	99
62	1,3-DINITROBENZENE	528-29-0	ALDRICH	97
63	1,4-DINITROBENZENE	100-25-4	ALDRICH	98
64	DINOCAP	39300-45-3	EPA/N	99
65	DINOSEB	88-85-7	EPA/N	97
66	DIOXATHION	78-34-2	EPA/N	89
67	5,5-DIPHENYLHYDANTOIN	57-41-0	ALDRICH	99
68	1,2-DIPHENYLHYDRAZINE	122-66-7	ALDRICH	97
69	DISULFOTON	298-04-4	EPA/N	98
70	EPN	2104-64-5	EPA/N	99
71	ETHION	563-12-2	EPA/N	99
72	ETHYL CARBAMATE	2104-64-5	EPA/N	99
73	ETHYLENE THIOUREA	563-12-2	EPA/N	99
74	ETHYL METHANESULFONATE	51-79-6	CHEM SERVICE	99
75	FAMPHUR	96-45-7	EPA/N	98
76	FENSULFOTHION	62-50-0	SIGMA	NA
77	FENTHION	52-85-7	EPA/N	98
78	FLUCHLORALIN	115-90-2	EPA/N	92
79	2-FLUOROACETAMIDE	55-38-9	EPA/N	95
80	HEXACHLOROPHENE	33245-39-5	EPA/N	100
81	HEXAMETHYL PHOSPHORAMIDE	640-19-7	ALDRICH	98
82	HYDROQUINONE	70-30-4	EPA/N	100
83	ISODRIN	680-31-9	ALDRICH	99
84	ISONICOTINIC ACID HYDRAZIDE	123-31-9	ALDRICH	99
85	ISOSAFROLE	465-73-6	EPA/N	100
86	KEPONE (CHLORDECONE)	54-85-3	ALDRICH	99
87	LEPTOPHOS	120-58-1	FLUKA	95 (d)
88	MALATHION	143-50-0	EPA/N	89 (e)
89	MALEIC ANHYDRIDE	21609-90-5	EPA/N	100
90	MALEIC HYDRAZIDE	121-75-5	EPA/N	98
91	MESTRANOL	72-33-3	ALDRICH	NA
92	METHAPYRILENE	91-80-5	ICN K&K	NA
93	METHOMYL	16752-77-5	EPA/N	100
94	p,p-METHOXYCHLOR	72-43-5	EPA/N	99
95	3-METHYLCHOLANTHRENE	56-49-5	P & B	99
96	4,4'-METHYLENEBIS(2-CHLOROANILINE)	101-14-4	CHEM SERVICE	NA
97	4,4'-METHYLENEBIS(N,N-DIMETHYL-ANILINE)	101-61-1	CHEM SERVICE	NA
98	METHYL METHANESULFONATE		ALDRICH	99
99	N-METHYL-N'-NITRO-N-NITROSOGUANIDINE	70-25-7	FLUKA	50 (f)
100	METHYL PARATHION	298-00-0	EPA/N	99

TABLE 2. (Continued)

NO.	SUBSTANCE	CAS NO.	SUPPLIER(a)	PURITY(b)
101	2-METHYLPHENOL	95-48-7	EPA/N	99
102	3-METHYLPHENOL	108-39-4	EPA/N	99
103	4-METHYLPHENOL	106-44-5	EPA/N	99
104	METHYLTHIOURACIL	56-04-2	ALDRICH	98
105	MEVINPHOS	7786-34-7	EPA/N	76
106	MEXACARBATE	315-18-4	EPA/N	99
107	MIREX	2385-85-5	EPA/N	100
108	MONOCROTOPHOS	6923-22-4	EPA/N	100
109	NALED	300-76-5	EPA/N	100
110	1,5-NAPHTHALENEDIAMINE	2243-62-1	P & B	96
111	1,4-NAPHTHOQUINONE	130-15-4	CHEM SERVICE	99
112	1-NAPHTHYLAMINE	134-32-7	SIGMA	90
113	2-NAPHTHYLAMINE	91-59-8	SIGMA	NA
114	1-NAPHTHYL-2-THIOUREA	86-88-4	EPA/N	95
115	NICLOSAMIDE	50-65-7	EPA/N	99
116	NICOTINE	54-11-5	ALDRICH	98
117	5-NITROACENAPHTHENE	602-87-9	EASTMAN	NA
118	4-NITROANILINE	100-01-6	EPA/S	NA
119	5-NITRO-o-ANISIDINE	99-59-2	P & B	NA
120	4-NITROBIPHENYL	92-93-3	SIGMA	NA
121	NITROFEN	1836-75-5	EPA/N	98
122	NITROGEN MUSTARD	51-75-2	ALDRICH	95
123	NITROGLYCERINE	55-63-0	ICI AMERICA	10 (g)
124	5-NITRO-O-TOLUIDINE	99-55-8	ALDRICH	99
125	4-NITROQUINOLINE-1-OXIDE	56-57-5	ALDRICH	98
126	N-NITROSODIBUTYLAMINE	924-16-3	EPA/N	98
127	N-NITROSODIETHANOLAMINE	1116-54-7	SIGMA	NA
128	N-NITROSODIETHYLAMINE	55-18-5	EPA/N	99
129	p-NITROSODIPHENYLAMINE	156-10-5	P & B	NA
130	N-NITROSO-N-ETHYLUREA	759-73-9	SIGMA	80 (h)
131	N-NITROSOMETHYLETHYLAMINE	10595-95-6	SIGMA	NA
132	N-NITROSO-N-METHYLUREA	684-93-5	SIGMA	75 (i)
133	N-NITROSO-N-METHYLURETHANE	615-53-2	P & B	95
134	N-NITROSOMORPHOLINE	59-89-2	SIGMA	NA
135	N-NITROSOPIPERIDINE	100-75-4	SIGMA	NA
136	N-NITROSOPYRROLIDINE	930-55-2	ALDRICH	99
137	OCTAMETHYL PYROPHOSPHORAMIDE	152-16-9	P & B	NA
138	OXYDEMETON-METHYL	301-12-2	EPA/N	54
139	4,4'-OXYDIANILINE	101-80-4	P & B	99
140	PARATHION	56-38-2	EPA/N	100
141	PENTACHLOROBENZENE	608-93-5	EPA/N	98
142	PENTACHLORONITROBENZENE	82-68-8	EPA/N	99
143	PHENACETIN	62-44-2	ALDRICH	97
144	PHENAZOPYRIDINE HYDROCHLORIDE	136-40-3	CHEM. DYNAMICS	98
145	PHENOBARBITAL	50-06-6	BCL	NA
146	1,2-PHENYLENEDIAMINE	95-54-5	ALDRICH	98
147	1,3-PHENYLENEDIAMINE	108-45-2	ALDRICH	99
148	1,4-PHENYLENEDIAMINE	106-50-3	ALDRICH	97
149	N-PHENYLTHIOUREA	103-85-5	ALDRICH	97
150	PHORATE	298-02-2	EPA/N	99

TABLE 2. (Continued)

NO.	SUBSTANCE	CAS NO.	SUPPLIER(a)	PURITY(b)
151	PHOSALONE	2310-17-0	EPA/N	98
152	PHOSMET	732-11-6	EPA/N	99
153	PHOSPHAMIDON	13171-21-6	EPA/N	66/29 (j)
154	PHTHALIC ANHYDRIDE	85-44-9	EPA/N	99
155	PIPERONYL SULFOXIDE	120-62-7	EPA/N	93
156	PRONAMIDE	23950-58-5	EPA/N	99
157	1,3-PROPANE SULTONE	1120-71-4	SIGMA	NA
158	PROPYLTHIOURACIL	51-52-5	ALDRICH	99
159	RESORCINOL	108-46-3	ALDRICH	NA
160	ROTENONE	83-79-4	EPA/N	97
161	SACCHARIN	81-07-2	FLUKA	99
162	SAFROLE	94-59-7	ALDRICH	97
163	STRYCHNINE	57-24-9	PIERCE CHEM	NA
164	SULFALLATE	95-06-7	EPA/N	100
165	TERBUFOS	13071-79-9	EPA/N	98
166	1,2,4,5-TETRACHLOROBENZENE	95-94-3	EPA/S	NA
167	2,3,4,6-TETRACHLOROPHENOL	58-90-2	EPA/N	86
168	TETRACHLORVINPHOS	961-11-5	EPA/N	100
169	TETRAETHYL DITHIOPYROPHOSPHATE	3689-24-5	POLYSCIENCE	QUAL
170	TETRAETHYL PYROPHOSPHATE	107-49-3	EPA/N	43 (k)
171	THIOACETAMIDE	62-55-5	ALDRICH	99
172	THIOFANOX	39196-18-4	EPA/N	99
173	THIONAZINE	297-97-2	EPA/N	99
174	TOLUENE DIISOCYANATE	584-84-9	FLUKA	80
175	o-TOLUIDINE	95-53-4	ALDRICH	NA
176	TRICHLORFON	52-68-6	EPA/N	99
177	2,4,5-TRICHLOROPHENOL	95-95-4	EPA/N	98
178	O,O,O-TRIETHYL PHOSPHOROTHIOATE	126-68-1	ICN K&K	NA
179	TRIFLURALIN	1582-09-8	EPA/N	100
180	2,4,5-TRIMETHYLANILINE	137-17-7	P & B	NA
181	TRIMETHYL PHOSPHATE	512-56-1	ALDRICH	99
182	1,3,5-TRINITROBENZENE	99-35-4	CHEM SERVICE	NA
183	TRIS(2,3-DIBROMOPROPYL) PHOSPHATE	126-72-7	ICN K&K	NA
184	TRI-p-TOLYL PHOSPHATE	78-32-0	EASTMAN	NA
185	WARFARIN	81-81-2	EPA/N	95

(a) BCR = Commission of the European Communities, Community Bureau of Reference
EPA/C = EPA Cinncinati respository
EPA/N = Neat compound obtained from EPA's main repository
EPA/S = pre-mixed solution obtained from EPA'S main repository
P & B = Pfaltz and Bauer

(b) NA = manufacter did not specify purity

(c) P=O is 54%, P=S is 39%

(d) cis/trans mix

(e) 11% water

(f) 50% water

(g) 90% hydrolactose

(h) 5% acetic acid

(i) 3% acetic acid

(j) trans is 66%, cis is 29%

(k) 55% triethyl phosphate

TABLE 3. INTERNAL STANDARDS USED FOR VOLATILE AND SEMIVOLATILE COMPOUND GC-MS ANALYSES

	Comments	Stock Concentration, ug/mL	Final Concentration, ug/mL
	VOLATILE		
Battelle Standards			
Benzene-D_6	99.6 Atom %	20	
Bromobenzene-D_5	99+ Atom %D	20,000	200
CLP Surrogate Standards			
4-Bromofluoro-benzene, BFB	Tuning Standard	20,000	200
1,2-Dichloro-ethane-D_4	99 Atom %D	20,000	200
Toluene-D_8	99.6 Atom %D	20,000	200
CLP Internal Standards			
Bromochloro-methane	--	20,000	200
1,4-Difluoro-benzene	99%	20,000	200
Chlorobenzene-D_5	99.5 Atom %D	20,000	200
	SEMIVOLATILE		
Decafluorotriphenyl-phosphine, DFTPP	Tuning Standard	4,000	40
CLP Internal Standards			
1,4-Dichloro-benzene-D_4		400	40
Naphthalene-D_8		400	40
Acenapthene-D_8		400	40
Phenanthrene-D_{10}		400	40
Chrysene-D_{12}		400	40
Perylene-D_{12}		400	40

TABLE 4. GC-MS ANALYSIS CONDITIONS

	Volatile Analytes	Semivolatile Analytes
	GC	
Column -	6 feet x 2 mm ID glass; packed with 1% SP1000 on Carbopack B 60/80 (Supelco)	30 meter x 0.25 mm fused silica with 0.25 micron methyl phenyl silicone film (J&W DB-5)
Carrier -	Helium at 30 mL/min, flow controlled	helium, pressure controlled at about 3 psi (about 30 m/sec at room temperature)
Sample -	1.5 uL, injected through septum of GC injector	2 uL injected splitless for 50 sec
Program -	45 C for 3 min, then program to 220 C at 8 C/min and hold for 15 min	room temperature for 4 min, then program to 300 C at 8 C/min and hold for 10 min
Injector -	250 C	300 C with fused silica evaporator cavity liner
	MS	
Mode -	electron impact at 70 eV; beam current about 0.3 mA	electron impact at 70 eV; beam current about 0.3 mA
Scan -	35 to 260 amu, 2.0 sec per scan	35 to 500 amu, 1.0 sec per scan
Transfer Oven -	250 C	300 C
Source Temperature -	not controllable	not controllable

TABLE 5. BFB AND DFTPP MS PERFORMANCE CRITERIA

Ion, m/e	Criterion
BFB	
50	15 to 40% of m/e 95
75	30 to 60% of m/e 95
95	Base Peak
96	5 to 9% of m/e 95
173	Less than 2% of m/e 174
174	Greater than 50% of m/e 95
175	5 to 9% of m/e 174
176	95 to 100% of m/e 174
177	5 to 9% of m/e 176
DFTPP	
51	30 to 60% of m/e 198
68	Less than 2% of m/e 69
70	Less than 2% of m/e 69
127	40 to 60% of m/e 198
197	Less than 1% of m/e 198
198	Base peak
199	5 to 9% of m/e 198
275	10 to 30% of m/e 198
365	Greater than 1% of m/e 198
441	Present but less than m/e 443
442	Greater than 40% of m/e 198
443	17 to 23% of m/e 442

TABLE 6 CLASSIFICATION OF ANALYTES CONSIDERED FOR GC-MS SUITABILITY TESTING

NO.	SUBSTANCE	LIST(a)		CAS NO.	RCRA NUMBER	MS LIB. NUMBER(b)	ANALYSIS GROUP(c)		
1	ACETALDEHYDE	8		75-07-0				O	
2	ACETONITRILE	8		75-05-8	U003	4	V		
3	ACETOPHENONE	8		98-86-2	U004	3031		S	
4	2-ACETYLAMINOFLUORENE	8		53-96-3	U005	19378		S	
5	ACETYL CHLORIDE	8		75-36-5	U006			O	
6	1-ACETYL-2-THIOUREA	8		591-08-2	P002	2799		S	
7	ACRYLAMIDE	8		79-06-1		204		S	
8	ACTINOMYCIN D		M	50-76-0	P124			O	
9	AFLATOXINS	8						O	
10	ALDICARB	8		116-06-3		14395		S	
11	ALLYL ALCOHOL	8		107-18-6	P005	69	V		
12	ALLYL CHLORIDE	8	M	107-05-1	U317	313	V		
13	2-AMINOANTHRAQUINONE		M	117-79-3	U264	19369		S	
14	AMINOAZOBENZENE		M	60-09-3	U257	15498		S	
15	4-AMINOBIPHENYL	8	M	92-67-1	U274	10938		S	
16	3-AMINO-9-ETHYLCARBAZOLE		M	132-32-1	U253			S	
17	1-AMINO-2-METHYLANTHRAQUINONE		M	82-28-0	U265				N
18	5-(AMINOMETHYL)-3-ISOXAZOLOL	8		2763-96-4	P007				N
19	AMITROLE	8		61-82-5	U011	455		S	
20	ANILAZINE		M	101-05-3	U333	25458		S	
21	ANILINE	8		62-53-3		840		S	
22	ANILINE HYDROCHLORIDE		M	142-04-1	U269	4112		O	
23	o-ANISIDINE HYDROCHLORIDE		M	134-29-2	U261			O	
24	o-ANISIDINE		M	90-04-0	U260	3249		S	
25	ARAMITE	8	M	140-57-8	U326	30755		S	
26	AURAMINE	8		492-80-8	U014			S	
27	AZASERINE	8		115-02-6	U015			O	
28	AZINOPHOS-ETHYL		M	2642-71-9	P150	31487			N
29	AZINPHOS-METHYL		M	86-50-0	P151	29421		S	
30	BARBAN		M	101-27-9	U280	23539		S	
31	BENOMYL		M	17804-35-2	U271	26964		S	
32	BENZ(C)ACRIDINE	8		225-51-4	U016				N
33	BENZAL CHLORIDE	8		98-87-3	U017	9279		O	
34	BENZENEARSONIC ACID	8		98-05-5				O	
35	BENZIDINE SULFATE		M	531-86-2				O	
36	7,8-BENZFLUORANTHENE	8		205-82-3					N
37	p-BENZOQUINONE	8		106-51-4	U197	1743		S	
38	BENZOTRICHLORIDE	8		98-07-7	U023	15052		O	
39	BENZYL CHLORIDE	8		100-44-7	P028	3603	V		
40	BIS-(2-CHLOROETHYL) SULFIDE	8	M	505-60-2	P158		V		
41	BIS(CHLOROMETHYL) ETHER	8		542-88-1		2309	V		
42	BROMOACETONE	8		598-31-2	P017		V		
43	BROMOXYNIL		M	1689-84-5	U272	25508		S	
44	BRUCINE	8		357-57-3	P018	34236		S	
45	2-BUTANONE PEROXIDE	8		1338-23-4	U160		V		
46	2-BUTANONE	8		78-93-3		223	V		
47	4-(BUTYLNITROSOAMINO)-1-BUTANOL		M	3817-11-6					N
48	CAPTAFOL		M	2425-06-1	U285	31611		S	
49	CAPTAN		M	133-06-2	U266	27860		S	

TABLE 6. (Continued)

NO.	SUBSTANCE	LIST(a)		CAS NO.	RCRA NUMBER	MS LIB. NUMBER(b)	ANALYSIS GROUP(c)			
50	CARBARYL		M	63-25-2	U279	16133		S		
51	CARBOFURAN		M	1563-66-2	U127	19005		S		
52	CARBON DISULFIDE	8		75-15-0			V			
53	CARBOPHENOTHION		M	786-19-6	U148			S		
54	CHLORAL(d)	8		75-87-6	U034	6678	V			N (d)
55	CHLORAMBUCIL	8		305-03-3	U035				O	
56	CHLORFENVINPHOS		M	470-90-6	P143	32264		S		
57	CHLOROACETALDEHYDE	8		107-20-0	P023	336			O	
58	4-CHLOROANILINE	8		106-47-8		3740		S		
59	CHLOROBENZILATE	8		510-15-6	U038	29969		S		
60	2-CHLOROETHANOL		M	107-07-3	P133	355	V			
61	5-CHLORO-2-METHYLANILINE		M	95-79-4	U329	5890		S		
62	CHLOROMETHYL METHYL ETHER	8		107-30-2	U046	356	V			
63	3-(CHLOROMETHYL)PYRIDINE HYDROCHLORIDE		M	6959-48-4	U319			S		
64	CHLORONAPHAZINE	8		494-03-1	U026					N
65	4-CHLORO-1,2-PHENYLENEDIAMINE		M	95-83-0	U306	6023		S		
66	4-CHLORO-1,3-PHENYLENEDIAMINE		M	5131-60-2	U305			S		
67	1-(2-CHLOROPHENYL)THIOUREA	8		5344-82-1	P026					M
68	CHLOROPRENE	8	M	126-99-8	U276	689	V			
69	3-CHLOROPROPIONITRILE	8		542-76-7	P027	745	V			
70	CITRUS RED NO. 2	8		6358-53-8						N
71	COAL TARS	8							O	
72	COUMAPHOS		M	56-72-4	P130	32529		S		
73	CREOSOTE	8		8001-58-9	U051				O	
74	p-CRESIDINE		M	120-71-8	U262	5213		S		
75	CROTONALDEHYDE	8		123-73-9					O	
76	CROTOXYPHOS		M	7700-17-6	U238	29095		S		
77	CUPFERRON		M	135-20-6	U290			S		
78	CYCASIN	8		14901-08-7					O	
79	CYCLOHEXIMIDE		M	66-81-9	P134	26033		S		
80	2-CYCLOHEXYL-4,6-DINITROPHENOL	8		131-89-5	P034	24443		S		
81	CYCLOPHOSPHAMIDE	8		50-18-0	U058			S		
82	2,4-D	8		94-75-7		18962			O	
83	DAUNOMYCIN	8		20830-81-3	U059				O	
84	DEMETON		M	8065-48-3	P155			S		
85	DIALLATE	8		2303-16-4	U062			S		
86	2,4-DIAMINOANISOLE SULFATE		M	39156-41-7	U307			S		
87	2,4-DIAMINOTOLUENE	8	M	95-80-7	U327	3162		S		
88	DIAZINON		M	333-41-5	U313	28285		S		
89	1,2:5,6-DIBENZACRIDINE	8		226-36-8						N
90	1,2:7,8-DIBENZACRIDINE	8		224-42-0				S		
91	3,4:5,6-DIBENZOCARBAZOLE	8		194-59-2						N
92	1,2:4,5-DIBENZOPYRENE	8		192-65-4				S		
93	DIBENZO(A,H)PYRENE	8		129-67-9						N
94	DIBENZO(A,I)PYRENE	8		189-55-9	U064					N
95	1,2-DIBROMO-3-CHLOROPROPANE	8		96-12-8		20858	V			
96	DIBROMOMETHANE	8		74-95-3			V			
97	DICHLONE		M	117-80-6	U299	19711		S		
98	DICHLORODIFLUOROMETHANE	8		75-71-8		2963	V			

TABLE 6. (Continued)

NO.	SUBSTANCE	LIST(a)		CAS NO.	RCRA NUMBER	MS LIB. NUMBER(b)	ANALYSIS GROUP(c)			
99	1,4-DICHLORO-2-BUTENE	8		764-41-0	U074	3297	V			
100	2,6-DICHLOROPHENOL	8		87-65-0		9673		S		
101	1,3-DICHLORO-2-PROPANOL	8		96-23-1			V			
102	DICHLOROVOS		M	62-73-7	P144	18944		S		
103	DICROTOPHOS		M	141-66-2	P146	21176		S		
104	1,2,3,4-DIEPOXYBUTANE	8		1464-53-5	U085	584	V			
105	DIETHYLARSINE	8		692-42-2	P038					N
106	1,2-DIETHYLHYDRAZINE	8		1615-80-1	U086	688				N
107	DIETHYLSTILBESTROL	8		56-53-1	U086			S		
108	DIETHYL SULFATE		M	64-67-5	U325	8164		S		
109	DIHYDROSAFROLE	8		56312-13-1	U090			S		
110	DIISOPROPYL FLUOROPHOSPHATE	8		55-91-4	P043					N
111	DIMETHOATE	8		60-51-5		20253		S		
112	3,3'-DIMETHOXYBENZIDINE	8		119-90-4	U091	22015		S		
113	DIMETHYLAMINOAZOBENZENE	8		60-11-7	U093	19680		S		
114	7,12-DIMETHYLBENZ(A)ANTHRACENE	8		57-97-6	U094	23504		S		
115	3,3'-DIMETHYLBENZIDINE	8		119-93-7	U095	17852		S		
116	DIMETHYLCARBAMOYL CHLORIDE	8		79-44-7	U097	1705			O	
117	3,3-DIMETHYL-1-(p-CHLOROPHENYL)TRIAZENE		M	7203-90-9						N
118	1,1-DIMETHYLHYDRAZINE	8		57-14-7	U098	90	V	S		
119	1,2-DIMETHYLHYDRAZINE	8		540-73-8	U099	92	V	S		
120	a,a-DIMETHYLPHENETHYLAMINE	8		122-09-8	P046	7163		S		
121	O,O-DIMETHYL-S-METHYL PHOSPHORODITHIOATE	8		3288-58-2	U087					N
122	1,2-DINITROBENZENE	8		99-65-0		10822		S		
123	1,3-DINITROBENZENE	8		528-29-0				S		
124	1,4-DINITROBENZENE	8		100-25-4		10823		S		
125	DINOCAP		M	39300-45-3	U284	32678		S		
126	DINOSEB	8		88-85-7		21460		S		
127	1,4-DIOXANE	8		123-91-1	U108	705	V			
128	DIOXATHION		M	78-34-2	P153	36614		S		
129	DIPHENYLAMINE	8							O	
130	5,5-DIPHENYLHYDANTOIN MONOSODIUM SALT		M	630-93-3					O	
131	5,5-DIPHENYLHYDANTOIN		M	57-41-0		22930		S		
132	1,2-DIPHENYLHYDRAZINE	8		122-66-7	U109	13398		S		
133	DISULFOTON	8		298-04-4		25449		S		
134	2,4-DITHIOBIURET	8		541-53-7	P049				O	
135	ENDOTHAL	8		129-67-9		20641			O	
136	EPICHLOROHYDRIN	8		106-89-8		816	V			
137	EPINEPHRINE (e)	8		51-43-4	P042	13317			O	(e)
138	EPN		M	2104-64-5	P141	29898		S		
139	ETHION		M	563-12-2	P154	33771		S		
140	ETHYL CARBAMATE	8		51-79-6	U238	746		S		
141	ETHYLENE BIS-DITHIOCARBAMATES	8		142-59-6					O	
142	ETHYLENE DIBROMIDE	8		106-93-4			V			
143	ETHYLENE OXIDE	8		75-21-8	U115	15	V			
144	ETHYLENE THIOUREA	8		96-45-7		1408		S		
145	ETHYLENIMINE	8		151-56-4	P054	11	V	S		
146	ETHYL METHACRYLATE	8		97-63-2	U118	2341	V			
147	ETHYL METHANESULFONATE	8		62-50-0	U119	3289		S		

TABLE 6. (Continued)

NO.	SUBSTANCE	LIST(a)		CAS NO.	RCRA NUMBER	MS LIB. NUMBER(b)	ANALYSIS GROUP(c)			
148	FAMPHUR	8		52-85-7	P097	30037		S		
149	FENSULFOTHION		M	115-90-2	P156	28592		S		
150	FENTHION		M	55-38-9		25683		S		
151	FLUCHLORALIN		M	33245-39-5	U330	32127		S		
152	2-FLUOROACETAMIDE	8		640-19-7	P057			S		
153	FLUOROACETIC ACID, SODIUM SALT	8		62-74-8					O	
154	FORMALDEHYDE	8		50-00-0					O	
155	FORMIC ACID	8		64-18-6					O	
156	FURATHIAZOLE		M	531-82-8	U251					N
157	GLYCIDALDEHYDE	8		765-34-4	U126				O	
158	HEXACHLOROPHENE	8		70-30-4	U132	34710		S		
159	HEXACHLOROPROPENE	8		1888-71-7	U243		V	S		
160	HEXAETHYL TETRAPHOSPHATE	8		757-58-4	P062					N
161	HEXAMETHYL PHOSPHORAMIDE		M	680-31-9	U312	12578		S		
162	HYDRAZINE	8		302-01-2	U133				O	
163	HYDROQUINONE		M	123-31-9		1900		S		
164	N-(2-HYDROXYETHYL)ETHYLENEIMINE		M	1072-52-2	U289		V			
165	2-HYDROXYPROPIONITRILE		M	78-97-7		203	V			
166	ISOBUTYL ALCOHOL	8		78-83-1		290	V			
167	ISODRIN	8		465-73-6	P060	32527		S		
168	ISONICOTINIC ACID HYDRAZIDE		M	54-85-3		5173		S		
169	ISOSAFROLE	8		120-58-1	U141	9490		S		
170	KEPONE	8		143-50-0		37389		S		
171	KETENE		M	463-51-4		8			O	
172	LASIOCARPINE	8		303-34-4	U143	34981			O	
173	LEPTOPHOS		M	21609-90-5	P140	34913		S		
174	MALACHITE GREEN		M	569-64-2	U254				O	
175	MALATHION		M	121-75-5	U324	30376		S		
176	MALEIC ANHYDRIDE	8		108-31-6	U147	1010		S		
177	MALEIC HYDRAZIDE	8		123-33-1		2041		S		
178	MALONONITRILE	8		109-77-3	U149	125	V			
179	MELPHALAN	8		148-82-3	U150				O	
180	MESTRANOL		M	72-33-3	U301	28817		S		
181	METHACRYLONITRILE	8		126-98-7	U152	140	V			
182	METHAPYRILENE	8		91-80-5	U155	24001		S		
183	METHOMYL	8		16752-77-5	P066	9649		S		
184	METHOXYCHLOR	8		72-43-5		31412		S		
185	2-METHYLAZIRIDINE	8		75-55-8	P067	60	V	S		
186	METHYL CHLOROCARBONATE	8		79-22-1	U156	849			O	
187	3-METHYLCHOLANTHRENE	8		56-49-5	U157	24784		S		
188	4,4-METHYLENEBIS(2-CHLOROANILINE)	8		101-14-4	U158	24450		S		
189	4,4'-METHYLENEBIS(2-METHYLANILINE)		M	838-88-0	U256					N
190	4,4'-METHYLENEBIS(N,N-DIMETHYL-ANILINE)		M	101-61-1	U255	23217		S		
191	METHYLHYDRAZINE	8		60-34-4	P068	23	V	S		
192	METHYL IODIDE	8		74-88-4	U138	5939	V			
193	METHYL ISOCYANATE	8		624-83-9	P064	58	V			
194	2-METHYLLACTONITRILE	8		75-86-5	P069	532	V			
195	METHYL MERCAPTAN	8		74-93-1		28	V			
196	METHYL METHACRYLATE	8		80-62-6	U162	1230	V			

TABLE 6. (Continued)

NO.	SUBSTANCE	LIST(a)		CAS NO.	RCRA NUMBER	MS LIB. NUMBER(b)	ANALYSIS GROUP(c)		
197	METHYL METHANESULFONATE	8					S		
198	2-METHYL-1-NITROANTHRAQUINONE		M	129-15-7		24614			N
199	N-METHYL-N-NITRO-N-NITROSOGUANIDINE	8		70-25-7	U163	6888	S		
200	METHYL PARATHION	8		298-00-0		24219	S		
201	2-METHYLPHENOL	8		95-48-7		1771	S		
202	3-METHYLPHENOL	8		108-39-4		1775	S		
203	4-METHYLPHENOL	8		106-44-5		1774	S		
204	METHYLTHIOURACIL	8		56-04-2	U164		S		
205	MEVINPHOS		M	7786-34-7	P131	19593	S		
206	MEXACARBATE		M	315-18-4	P128	19119	S		
207	MIREX		M	2385-85-5	U297	38190	S		
208	MITOMYCIN C	8		50-07-7	U010	30752		O	
209	MONOCROTALINE		M	315-22-0		30044		O	
210	MONOCROTOPHOS		M	6923-22-4	P147	19397	S		
211	NALED		M	300-76-5	U309	33491	S		
212	1,5-NAPHTHALENEDIAMINE		M	2243-62-1	U298		S		
213	1,4-NAPHTHOQUINONE	8		130-15-4	U166	8839	S		
214	1-NAPHTHYLAMINE	8		134-32-7	U167	6207	S		
215	2-NAPHTHYLAMINE	8		91-59-8	U168		S		
216	1-NAPHTHYL-2-THIOUREA	8		86-88-4	P072	16231	S		
217	NICLOSAMIDE		M	50-65-7	U321		S		
218	NICOTINE	8		54-11-5	P075	9534	S		
219	NIFURTHIAZOL		M	3570-75-0					N
220	NIRIDAZOLE		M	61-57-4	U293				N
221	NITHIAZIDE		M	139-94-6	U335				N
222	5-NITROACENAPHTHENE		M	602-87-9	U250		S		
223	4-NITROANILINE	8		100-01-6		5358	S		
224	5-NITRO-o-ANISIDINE		M	99-59-2	U263	10836	S		
225	4-NITROBIPHENYL		M	92-93-3	U275	15854	S		
226	NITROFEN		M	1836-75-5	U288	26234	S		
227	NITROGEN MUSTARD	8	M	51-75-2	P132		S		
228	NITROGEN MUSTARD N-OXIDE	8		302-70-5				O	
229	NITROGLYCERINE	8		55-63-0	P081	19986	S		
230	5-NITRO-O-TOLUIDINE	8		99-55-8	U181	7752	S		
231	4-NITROQUINOLINE-1-OXIDE	8		56-57-5			S		
232	N-NITROSODIBUTYLAMINE	8		924-16-3		8954	S		
233	N-NITROSODIETHANOLAMINE	8		1116-54-7	U173		S		
234	N-NITROSODIETHYLAMINE	8		55-18-5		1410	S		
235	p-NITROSODIPHENYLAMINE		M	156-10-5	U287	15632	S		
236	N-NITROSO-N-ETHYLUREA	8		759-73-9	U176	2763	S		
237	N-NITROSOMETHYLETHYLAMINE	8		10595-95-6			S		
238	N-NITROSO-N-METHYLUREA	8		684-93-5	U177	1505	S		
239	N-NITROSO-N-METHYLURETHANE	8		615-53-2	U178	4481	S		
240	N-NITROSOMETHYLVINYLAMINE	8		4549-40-0	P084	557			N
241	N-NITROSOMORPHOLINE	8		59-89-2			S		
242	N-NITROSONORNICOTINE	8		16543-55-8					N
243	N-NITROSOPIPERIDINE	8		100-75-4	U176	2332	S		
244	N-NITROSOPYRROLIDINE	8		930-55-2		1215	S		
245	N-NITROSOSARCOSINE	8		13256-22-9				O	

TABLE 6. (Continued)

NO.	SUBSTANCE	LIST(a)		CAS NO.	RCRA NUMBER	MS LIB. NUMBER(b)	ANALYSIS GROUP(c)		
246	OCTAMETHYL PYROPHOSPHORAMIDE	8		152-16-9	P085	26664	S		
247	OXYDEMETON-METHYL		M	301-12-2	P157		S		
248	4,4'-OXYDIANILINE		M	101-80-4	U303	15962	S		
249	PARALDEHYDE	8		123-63-7	U182	4522		O	
250	PARATHION ETHYL	8		56-38-2		27067	S		
251	PENTACHLOROBENZENE	8		608-93-5		22534	S		
252	PENTACHLOROETHANE	8		76-01-7		16044	V		
253	PENTACHLORONITROBENZENE	8		82-68-8		27251	S		
254	PEROXYACETIC ACID		M	79-21-0	U304			O	
255	PHENACETIN	8		62-44-2	U187	12523	S		
256	PHENAZOPYRIDINE HYDROCHLORIDE		M	136-40-3	U320		S		
257	PHENESTERIN		M	3546-10-9	U252			O	
258	PHENOBARBITAL		M	50-06-6	U268	20538	S		
259	PHENYL DICHLOROARSINE	8		696-28-6				O	
260	1,2-PHENYLENEDIAMINE	8		95-54-5		1744	S		
261	1,3-PHENYLENEDIAMINE	8		108-45-2			S		
262	1,4-PHENYLENEDIAMINE	8		106-50-3		1746	S		
263	N-PHENYLTHIOUREA	8		103-85-5	P093	7762	S		
264	PHORATE	8		298-02-2		23956	S		
265	PHOSACETIM		M	4104-14-7	P142	33254			N
266	PHOSALONE	8		2310-17-0			S		
267	PHOSMET		M	732-11-6		29423	S		
268	PHOSPHAMIDON		M	13171-21-6	P145	27796	S		
269	PHTHALIC ANHYDRIDE	8		85-44-9	U190	7118	S		
270	2-PICOLINE	8		109-06-8	U191	843	V		
271	PIPERONYL SULFOXIDE		M	120-62-7	U270	29987	S		
272	POLYBROMINATED BIPHENYLS		M	59536-65-1	U136			O	
273	POLYCHLORINATED BIPHENYLS	8		1336-36-3				O	
274	PRONAMIDE	8		23950-58-5		23303	S		
275	1,3-PROPANE SULTONE	8		1120-71-4	U193	3126	S		
276	PROPARGYL ALCOHOL	8		107-19-7	P102	49	V		
277	b-PROPIOLACTONE		M	57-57-8	U302	214	V		
278	PROPIONITRILE	8		107-12-0	P101	44	V		
279	n-PROPYLAMINE	8		107-10-8	U194	59	V		
280	PROPYLTHIOURACIL	8	M	51-52-5	U334	11178	S		
281	PYRIDINE	8		110-86-1	U196	349	V		
282	RESERPINE	8		50-55-5	U200	38864		O	
283	RESORCINOL	8		108-46-3		1898	S		
284	ROTENONE		M	83-79-4	U273	34232	S		
285	SACCHARIN	8		81-07-2	U202	13296	S		
286	SAFROLE	8		94-59-7	U203	9487	S		
287	SEMICARBAZIDE		M	57-56-7				O	
288	SILVEX	8		93-72-1		24803		O	
289	STREPTOZOTOCIN	8		18883-66-4	U206			O	
290	STRYCHNINE	8		57-24-9		30807	S		
291	STYRENE		M	100-42-5	U323		V		
292	SULFALLATE		M	95-06-7	U277	19398	S		
293	2,4,5-T	8		93-76-5		23266		O	
294	2,3,7,8-TCDD	8		1746-01-6		29647		O	

TABLE 6. (Continued)

NO.	SUBSTANCE	LIST(a)		CAS NO.	RCRA NUMBER	MS LIB. NUMBER(b)	ANALYSIS GROUP(c)			
295	TERBUFOS		M	13071-79-9	P149	26848		S		
296	1,2,4,5-TETRACHLOROBENZENE	8		95-94-3		18165		S		
297	1,1,1,2-TETRACHLOROETHANE	8		630-20-6			V			
298	2,3,4,6-TETRACHLOROPHENOL	8		58-90-2		20418		S		
299	TETRACHLORVINPHOS		M	961-11-5	U308	32646		S		
300	TETRAETHYL DITHIOPYROPHOSPHATE	8		3689-24-5	P109	29889		S		
301	TETRAETHYL PYROPHOSPHATE	8		107-49-3		27066		S		
302	TETRANITROMETHANE	8		509-14-8	P112	15217	V	S		
303	THIOACETAMIDE	8		62-55-5	U128	299		S		
304	4,4'-THIODIANILINE		M	139-65-1	U258					N
305	THIOFANOX	8		39196-18-4	P045	18701		S		
306	THIONAZINE	8		297-97-2	P040	22545		S		
307	THIOPHENOL	8		108-98-5	P104	1903	V	S		
308	THIOSEMICARBAZIDE	8		79-19-6	P116	804			O	
309	THIOUREA	8		62-56-6	U219	308			O	
310	THIRAM	8		137-26-8	U244	21619			O	
311	TOLUENE DIISOCYANATE	8		584-84-9	U223	11916		S		
312	o-TOLUIDINE	8	M	95-53-4	U328	1709		S		
313	TRICHLORFON		M	52-68-6	P139	23511		S		
314	TRICHLOROMETHANESULFENYL CHLORIDE	8		594-42-3	P118				O	
315	2,4,5-TRICHLOROPHENOL	8		95-95-4		15448		S		
316	1,2,3-TRICHLOROPROPANE	8		96-18-4			V			
317	TRICRESYL PHOSPHATE(f)		M	78-30-8	U311	32908		S		(f)
318	O,O,O-TRIETHYL PHOSPHOROTHIOATE	8		126-68-1				S		
319	TRIFLURALIN		M	1582-09-8	U332	30852		S		
320	2,4,5-TRIMETHYLANILINE		M	137-17-7	U259			S		
321	TRIMETHYL PHOSPHATE		M	512-56-1	U310	5619		S		
322	1,3,5-TRINITROBENZENE	8		99-35-4	U234			S		
323	TRIS(1-AZRIDINYL) PHOSPHINE SULFIDE	8								N
324	TRIS(2,3-DIBROMOPROPYL) PHOSPHATE	8		126-72-7	U235	39315		S		
325	TRYPAN BLUE	8		72-57-1	U236				O	
326	URACIL MUSTARD	8		66-75-1	U237					N
327	WARFARIN	8		81-81-2	P001	28644		S		
328	ZIRAM		M	137-30-4	U336	28389			O	

(a) 8 = Appendix VIII; M = Michigan list

(b) EPA/NIH Mass spectral data base, 1983 version, 39763 mass spectra.

(c) V= volatile, method 8240
S= semivolatile, method 8270
O= omitted a priori
N= not commercially available
Analytes indicated as both S and V were tested in both categories

(d) Chloral not commercially available but used chloral hydrate in volatiles testing

(e) Epinephrine (Pfaltz and \Bauer 99% purity) was found to be insoluble in any organic solvent suitable for semivolatile method injection and was was omitted from further testing.

(f) Tricresyl phosphate, a mixture of isomers, was not used.
Tri-p-tolyl phosphate was substituted in semivolatile testing.

TABLE 7. ANALYTES OMITTED A PRIORI FROM GC-MS SUITABILITY TESTING

NO.	SUBSTANCE	LIST(a)	CAS NO.	REASON FOR OMMISSION	SUGGESTED ANALYTICAL APPROACH FOR FUTURE WORK
1	ACETALDEHYDE	8	75-07-0	ALDEHYDE	DERIV/HPLC-UV(b)
2	ACETYL CHLORIDE	8	75-36-5	HYDROLYTICALLY UNSTABLE	NONE
3	ACTINOMYCIN D	M	50-76-0	NONVOLATILE	HPLC
4	AFLATOXINS	8	98-05-5	NONVOLATILE	HPLC-FLUOR(b)
5	ANILINE HYDROCHLORIDE	M	142-04-1	REDUNDANT	
6	o-ANISIDINE HYDROCHLORIDE	M	134-29-2	REDUNDANT	
7	AZASERINE	8	115-02-6	ACID	DERIV/GC-MS OR HPLC
8	BENZAL CHLORIDE	8	98-87-3	HYDROLYTICALLY UNSTABLE	NONE
9	BENZENEARSONIC ACID	8	98-05-5	ACID	HPLC
10	BENZIDINE SULFATE	M	531-86-2	REDUNDANT WITH PRIORITY POLLUTANT	
11	BENZOTRICHLORIDE	8	98-07-7	HYDROLYTICALLY UNSTABLE	NONE
12	CHLORAMBUCIL	8	305-03-3	ACID	DERIV/GC-MS OR HPLC
13	CHLOROACETALDEHYDE	8	107-20-0	ALDEHYDE	DERIV/HPLC-UV(b)
14	COAL TARS	8	20830-81-3	NONSPECIFIC MIXTURE	HPLC
15	CREOSOTE	8	8001-58-9	NONSPECIFIC MIXTURE	HPLC
16	CROTONALDEHYDE	8	123-73-9	ALDEHYDE	DERIV/HPLC-UV(b)
17	CYCASIN	8	14901-08-7	NONVOLATILE	HPLC/POST COLUMN DERIV.
18	2,4-D	8	94-75-7	ACID	DERIV/GC-MS(b)
19	DAUNOMYCIN	8	20830-81-3	NONVOLATILE	HPLC
20	DIMETHYLCARBAMOYL CHLORIDE	8	79-44-7	HYDROLYTICALLY UNSTABLE	
21	DIPHENYLAMINE	8	62-74-8	(c)	
22	5,5-DIPHENYLHYDANTOIN MONOSODIUM SALT	M	630-93-3	REDUNDANT WITH No. 131 OF TABLE 6	
23	2,4-DITHIOBIURET	8	541-53-7	INAPPROPRIATE FOR ORGANIC COMPOUND GROUPS	NON-CHROMATOGRAPHIC METHOD
24	ENDOTHAL	8	129-67-9	ACID	DERIV/GC-MS
25	EPINEPHRINE	8	51-43-4	NOT SOLUBLE IN ORGANIC SOLVENTS	ION CHROMATOGRAPHY OR HPLC
26	ETHYLENE BIS-DITHIOCARBAMATES	8	142-59-6	NONVOLATILE AS SALTS, UNSTABLE AS FREE ACID	DERIV GC, HPLC, OR INDIRECT GC(d)
27	FLUOROACETIC ACID, SODIUM SALT	8	62-74-8	ACID	DERIV GC-MS
28	FORMALDEHYDE	8	50-00-0	ALDEHYDE	DERIV/HPLC-UV(b)
29	FORMIC ACID	8	64-18-6	ACID	ION CHROMATOGRAPHY
30	GLYCIDALDEHYDE	8	765-34-4	ALDEHYDE	DERIV/HPLC-UV(b)
31	HYDRAZINE	8	302-01-2	INAPPROPRIATE FOR ORGANIC COMPOUND GROUPS	
32	KETENE	M	463-51-4	SPECIAL CHEMICAL STABILITY PROBLEM	
33	LASIOCARPINE	8	303-34-4	ACID	HPLC
34	MALACHITE GREEN	M	569-64-2	NONVOLATILE, QUATERNARY AMINE	HPLC

TABLE 7. (Continued)

NO.	SUBSTANCE	LIST(a)	CAS NO.	REASON FOR OMMISSION	SUGGESTED ANALYTICAL APPROACH FOR FUTURE WORK
35	MELPHALAN	8	148-82-3	ACID	HPLC
36	METHYL CHLOROCARBONATE	8	79-22-1	HYDROLYTICALLY UNSTABLE	
37	MITOMYCIN C	8	50-07-7	NONVOLATILE	HPLC
38	MONOCROTALINE	M	315-22-0	NONVOLATILE	HPLC
39	NITROGEN MUSTARD N-OXIDE	8	302-70-5	THERMOLABILE	HPLC/ECD
40	N-NITROSOSARCOSINE	8	13256-22-9	ACID	HPLC OR DERIV GC-MS
41	PARALDEHYDE	8	123-63-7	ALDEHYDE	DERIV/HPLC-UV(b)
42	PEROXYACETIC ACID	M	79-21-0	ACID, UNSTABLE	
43	PHENESTERIN	M	3546-10-9	NONVOLATILE	HPLC
44	PHENYL DICHLOROARSINE	8	696-28-6	HYDROLYTICALLY UNSTABLE	
45	POLYBROMINATED BIPHENYLS	M	59536-65-1	INAPPROPRIATE FOR THE PRESENT SCOPE	(b)
46	POLYCHLORINATED BIPHENYLS	8	1336-36-3	INAPPROPRIATE FOR THE PRESENT SCOPE	(b)
47	RESERPINE	8	50-55-5	NONVOLATILE	HPLC
48	SEMICARBAZIDE	M	57-56-7	INAPPROPRIATE FOR THE PRESENT SCOPE	
49	SILVEX	8	93-72-1	ACID	DERIV GC-MS
50	STREPTOZOTOCIN	8	18883-66-4	NONVOLATILE	HPLC
51	2,4,5-T	8	93-76-5	ACID	DERIV GC-MS
52	2,3,7,8-TCDD	8	1746-01-6	WELL CHARACTERIZED BY OTHER EPA METHODS	(b)
53	THIOSEMICARBAZIDE	8	79-19-6	INAPPROPRIATE FOR ORGANIC COMPOUND GROUPS	
54	THIOUREA	8	62-56-6	INAPPROPRIATE FOR ORGANIC COMPOUND GROUPS	
55	THIRAM	8	137-26-8	HYDROLYTICALLY AND THERMALLY UNSTABILE	INDIRECT GC(d)
56	TRICHLOROMETHANESULFENYL CHLORIDE	8	594-42-3	HYDROLYTICALLY UNSTABLE	
57	TRYPAN BLUE	8	72-57-1	NONVOLATILE	HPLC
58	ZIRAM	M	137-30-4	NONVOLATILE	HPLC

(a) 8 = Appendix VIII; M = Michigan List

(b) Partially or fully demonstrated method for selected matrices already exists.

(c) Diphenylamine has been well characterized by GC-MS since the priority pollutant N-nitrodiphenylamine has been thoroughly demonstrated to quantitatively decompose to diphenylamine upon GC injection.

(d) This family of analytes have been successfully determined in aqueous media by GC-Hall/Sulfur analysis of carbon disulfide decomposition product.

TABLE 8. VOLATILE AND SEMIVOLATILE ANALYTES NOT OBTAINABLE IN TIME FOR INCLUSION

NUMBER	SUBSTANCE	LIST(a)	CAS NO.
1	1-AMINO-2-METHYLANTHRAQUINONE	M	82-28-0
2	5-(AMINOMETHYL)-3-ISOXAZOLOL	8	2763-96-4
3	AZINOPHOS-ETHYL	M	2642-71-9
4	BENZ(C)ACRIDINE	8	225-51-4
5	7,8-BENZFLUORANTHENE	8	205-82-3
6	4-(BUTYLNITROSOAMINO)-1-BUTANOL	M	3817-11-6
7	CHLORAL (b)	8	75-87-6
8	CHLORONAPHAZINE	8	494-03-1
9	1-(2-CHLOROPHENYL)THIOUREA	8	5344-82-1
10	CITRUS RED NO. 2	8	6358-53-8
11	1,2:5,6-DIBENZACRIDINE	8	226-36-8
12	3,4:5,6-DIBENZOCARBAZOLE	8	194-59-2
13	DIBENZO(A,I)PYRENE (c)	8	189-55-9
14	DIBENZO(A,H)PYRENE	8	129-67-9
15	DIETHYLARSINE	8	692-42-2
16	1,2-DIETHYLHYDRAZINE	8	1615-80-1
17	DIISOPROPYL FLUOROPHOSPHATE	8	55-91-4
18	3,3-DIMETHYL-1-(p-CHLOROPHENYL)TRIAZENE	M	7203-90-9
19	O,O-DIMETHYL-S-METHYL PHOSPHORODITHIOATE	8	3288-58-2
20	FURATHIAZOLE	M	531-82-8
21	HEXAETHYL TETRAPHOSPHATE	8	757-58-4
22	4,4'-METHYLENEBIS(2-METHYLANILINE)	M	838-88-0
23	2-METHYL-1-NITROANTHRAQUINONE	M	129-15-7
24	NIFURTHIAZOL	M	3570-75-0
25	NIRIDAZOLE	M	61-57-4
26	NITHIAZIDE	M	139-94-6
27	N-NITROSOMETHYLVINYLAMINE	8	4549-40-0
28	N-NITROSONORNICOTINE	8	16543-55-8
29	PHOSACETIM	M	4104-14-7
30	4,4'-THIODIANILINE	M	139-65-1
31	TRIS(1-AZRIDINYL) PHOSPHINE SULFIDE	8	
32	URACIL MUSTARD	8	66-75-1

(a) 8 = Appendix VIII; M = Michigan list

(b) Chloral hydrate was substituted for chloral

(c) Judged cost prohibitive for this program.

TABLE 9. VOLATILE ANALYTES TESTED FOR GC-MS SUITABILITY

NO.	SUBSTANCE	ST(a)		CAS NO.	RCRA NUMBER	STATUS CODE(b)
1	ACETONITRILE	8		75-05-8	U003	S
2	ALLYL ALCOHOL	8		107-18-6	P005	S
3	ALLYL CHLORIDE	8	M	107-05-1	U317	S
4	BENZYL CHLORIDE	8		100-44-7	P028	S
5	BIS-(2-CHLOROETHYL) SULFIDE	8	M	505-60-2	P158	LR
6	BIS(CHLOROMETHYL) ETHER	8		542-88-1		ND
7	BROMOACETONE	8		598-31-2	P017	S
8	2-BUTANONE PEROXIDE	8		1338-23-4	U160	ND
9	2-BUTANONE	8		78-93-3		S
10	CARBON DISULFIDE	8		75-15-0		S
11	CHLORAL HYDRATE	8		75-87-6	U034	LR
12	2-CHLOROETHANOL		M	107-07-3	P133	LR
13	CHLOROMETHYL METHYL ETHER	8		107-30-2	U046	ND
14	CHLOROPRENE	8	M	126-99-8	U276	S
15	3-CHLOROPROPIONITRILE	8		542-76-7	P027	S
16	1,2-DIBROMO-3-CHLOROPROPANE	8		96-12-8		S
17	DIBROMOMETHANE	8		74-95-3		S
18	1,4-DICHLORO-2-BUTENE	8		764-41-0	U074	S
19	DICHLORODIFLUOROMETHANE	8		75-71-8		S
20	1,3-DICHLORO-2-PROPANOL	8		96-23-1		S
21	1,2,3,4-DIEPOXYBUTANE	8		1464-53-5	U085	S
22	1,1-DIMETHYLHYDRAZINE	8		57-14-7	U098	ND
23	1,2-DIMETHYLHYDRAZINE	8		540-73-8	U099	ND
24	1,4-DIOXANE	8		123-91-1	U108	S
25	EPICHLOROHYDRIN	8		106-89-8		S
26	ETHYLENE DIBROMIDE	8		106-93-4		S
27	ETHYLENE OXIDE	8		75-21-8	U115	S
28	ETHYLENIMINE	8		151-56-4	P054	ND
29	ETHYL METHACRYLATE	8		97-63-2	U118	S
30	HEXACHLOROPROPENE	8		1888-71-7	U243	ND
31	N-(2-HYDROXYETHYL)ETHYLENEIMINE		M	1072-52-2	U289	ND
32	2-HYDROXYPROPIONITRILE		M	78-97-7		LR
33	ISOBUTYL ALCOHOL	8		78-83-1		S
34	MALONONITRILE	8		109-77-3	U149	S
35	METHACRYLONITRILE	8		126-98-7	U152	S
36	2-METHYLAZIRIDINE	8		75-55-8	P067	ND
37	METHYLHYDRAZINE	8		60-34-4	P068	ND
38	METHYL IODIDE	8		74-88-4	U138	S
39	METHYL ISOCYANATE	8		624-83-9	P064	ND
40	2-METHYLLACTONITRILE	8		75-86-5	P069	ND
41	METHYL MERCAPTAN	8		74-93-1		ND
42	METHYL METHACRYLATE	8		80-62-6	U162	S
43	PENTACHLOROETHANE	8		76-01-7		S
44	2-PICOLINE	8		109-06-8	U191	S
45	PROPARGYL ALCOHOL	8		107-19-7	P102	LR

TABLE 9. (Continued)

NO.	SUBSTANCE	LIST(a)	CAS NO.	RCRA NUMBER	STATUS CODE(b)
46	b-PROPIOLACTONE	M	57-57-8	U302	S
47	PROPIONITRILE	8	107-12-0	P101	S
48	n-PROPYLAMINE	8	107-10-8	U194	LR
49	PYRIDINE	8	110-86-1	U196	S
50	STYRENE	M	100-42-5	U323	S
51	1,1,1,2-TETRACHLOROETHANE	8	630-20-6		S
52	TETRANITROMETHANE	8	509-14-8	P112	ND
53	THIOPHENOL	8	108-98-5	P104	ND
54	1,2,3-TRICHLOROPROPANE	8	96-18-4		S

(a) 8 = Appendix VIII; M = Michigan list

(b) LR: low response factor
S: suitable for GC/MS analysis
ND: not detected in GC/MS data

TABLE 10. GC AND MS CHARACTERISTICS FOR VOLATILE ANALYTES THAT WERE DETECTED

NO.	SUBSTANCE	LIST(a)	CAS NO.	RCRA NUMBER	NBS LIB. NUMBER(b)	RT (MIN)	RRI(c)	RECOMMENDED QUAN ION	RECOMMENDED SEARCH IONS IN DECENDING OF IMPORTANCE (RELATIVE ABUNDANCE)	ORDER	RESPONSE FACTOR(d)
1	ACETONITRILE	8	75-05-8	U003	4	3.97	0.23	41	41 (100) 40 (53) 39 (20)		0.34
2	ALLYL ALCOHOL	8	107-18-6	P005	69	9.77	0.57	57	57 (100) 58 (20) 39 (30)		0.18
3	ALLYL CHLORIDE	8 M	107-05-1	U317	313	8.83	0.52	76	76 (30) 41 (100) 39 (65) 78 (10)		0.11
4	BENZYL CHLORIDE	8	100-44-7	P028	3603	29.50	1.73	91	91 (100) 126 (20) 65 (14) 128 (5)		0.56
5	BIS-(2-CHLOROETHYL) SULFIDE	8 M	505-60-2	P158		33.53	1.96	109	109 (100) 111 (35) 158 (20) 160 (12)		0.02(f)
6	BROMOACETONE	8	598-31-2	P017		16.33	0.96	136	43 (100) 136 (7) 138 (7) 93 (6) 95	(6)	0.03
7	2-BUTANONE	8	78-93-3		223	12.20	0.71	72	43 (100) 72 (23)		0.17
8	CARBON DISULFIDE	8	75-15-0		310	7.47	0.44	76	76 (100) 78 (10) 44 (12)		0.68
9	CHLORAL HYDRATE	8	75-87-6	U034	6678	15.77	0.92	82	82 (90) 44 (100) 84 (70) 86 (35) 111	(33)	0.009(f)
10	2-CHLOROETHANOL	M	107-07-3	P133	355	12.93	0.76	49	49 (12) 44 (100) 43 (60) 51 (9) 80	(5)	0.009(f)
11	CHLOROPRENE	8 M	126-99-8	U276	698	14.77	0.87	53	53 (100) 88 (60) 90 (20) 51 (23)		0.11
12	3-CHLOROPROPIONITRILE	8	542-76-7	P027	745	17.37	1.02	54	54 (95) 49 (100) 89 (20) 91 (8)		0.17
13	1,2-DIBROMO-3-CHLOROPROPANE	8	96-12-8		20858	27.23	1.60	157	157 (87) 75 (100)155 (63) 77 (30)		0.26
14	DIBROMOMETHANE	8	74-95-3		11361	12.53	0.73	93	93 (100) 174 (80) 95 (82) 172 (40) 176	(36)	0.31
15	1,4-DICHLORO-2-BUTENE	8	764-41-0	U074	3297	22.73	1.33	75	75 (80) 53 (100) 77 (23) 124 (10) 89	(35)	0.14
16	DICHLORODIFLUOROMETHANE	8	75-71-8		2963	2.47	0.14	85	85 (100) 87 (35) 101 (10) 103 (7)		0.18
17	1,3-DICHLORO-2-PROPANOL	8	96-23-1		3829	21.83	1.28	79	79 (100) 43 (85) 81 (33) 49 (27)		0.20
18	1,2,3,4-DIEPOXYBUTANE	8	1464-53-5	U085	584	14.87	0.87	55	55 (100) 57 (15) 56 (9)		0.14
19	1,4-DIOXANE	8	123-91-1	U108	705	13.70	0.80	88	88 (100) 58 (70) 43 (30) 57 (23)		0.24
20	EPICHLOROHYDRIN	8	106-89-8		816	13.10	0.77	57	57 (100) 49 (22) 62 (15) 51 (8)		0.34
21	ETHYLENE DIBROMIDE	8	106-93-4		13846	18.40	1.08	107	107 (100) 109 (95) 93 (6) 188 (3)		0.56
22	ETHYLENE OXIDE	8	75-21-8	U115	15	1.30	0.08	44	44 (100) 43 (20) 42 (15)		0.19
23	ETHYL METHACRYLATE	8	97-63-2	U118	2341	23.53	1.38	69	69 (100) 41 (70) 99 (20) 86 (15) 114	(5)	0.58
24	2-HYDROXYPROPIONITRILE	M	78-97-7		203	18.97	1.11	44	44 (100) 43 (60) 42 (15) 53 (5)		0.009(f)
25	ISOBUTYL ALCOHOL	8	78-83-1		290	13.80	0.81	43	43 (100) 41 (66) 42 (60) 74 (9)		0.28
26	MALONONITRILE	8	109-77-3	U149	125	19.60	1.15	66	66 (100) 39 (14) 65 (10) 38 (11)		0.15
27	METHACRYLONITRILE	8	126-98-7	U152	140	12.37	0.72	41	41 (100) 67 (50) 39 (51) 52 (22) 66	(20)	0.34
28	METHYL IODIDE	8	74-88-4	U138	5939	5.37	0.31	142	142 (100) 127 (37) 141 (15)		0.51
29	METHYL METHACRYLATE	8	80-62-6	U162	1230	19.77	1.16	69	69 (80) 41 (100)100 (30) 39 (47)		0.18
30	PENTACHLOROETHANE(e)	8	76-01-7		16044	24.83	1.46	167	167 (77) 130 (79) 132 (77) 165 (57) 169	(37)	0.12
31	2-PICOLINE	8	109-06-8	U191	843	23.20	1.36	93	93 (100) 66 (36) 92 (27) 78 (17)		0.43
32	PROPARGYL ALCOHOL	8	107-19-7	P102	49	10.77	0.63	55	55 (100) 39 (25) 38 (15) 53 (10)		0.005(f)
33	b-PROPIOLACTONE	M	57-57-8	U302	214	13.00	0.76	42	42 (100) 43 (32) 44 (5)		0.08
34	PROPIONITRILE	8	107-12-0	P101	44	8.53	0.50	54	54 (100) 52 (17) 55 (16) 40 (7)		0.26
35	n-PROPYLAMINE	8	107-10-8	U194	81	23.00	1.35	59	59 (100) 41 (47) 39 (25)		0.01(f)
36	PYRIDINE	8	110-86-1	U196	349	18.57	1.09	79	79 (100) 52 (73) 51 (33) 50 (25)		0.37
37	STYRENE	M	100-42-5	U323	1625	30.83	1.81	104	104 (100) 103 (50) 78 (42) 51 (25) 77	(20)	0.67
38	1,1,1,2-TETRACHLOROETHANE	8	630-20-6		10335	20.33	1.19	131	131 (100) 133 (97) 117 (70) 119 (68) 95	(33)	0.31

TABLE 10. (Continued)

NO	SUBSTANCE	LIST(a)	CAS NO.	RCRA NUMBER	NBS LIB. NUMBER(b)	RT (MIN)	RRI(c)	RECOMMENDED QUAN ION	RECOMMENDED SEARCH IONS IN DECENDING ORDER OF IMPORTANCE (RELATIVE ABUNDANCE)	RESPONSE FACTOR(d)
39	1,2,3-TRICHLOROPROPANE	8	96-18-4		6685	22.20	1.30	75	75 (100) 77 (30) 110 (33) 112 (20) 97 (17)	0.62

(a) 8 = Appendix VIII; M = Michigan list

(b) EPA/NIH Mass Spectral Data Base, 1983 version, 39,763 mass spectra.

(c) Retention index relative to benzene-D6.

(d) Response factor = $\frac{\text{Area (quant ion)} \times \text{Amount benzene-D6}}{\text{Area (m/e 84, benzene-D6)} \times \text{Amount analyte}}$

(e) The base peak at m/e 117 was not used due to an interferance at that mass with a nearly coeluting internal standard, chlorobenzene-D5

(f) Response factor judged to be too low (i.e. less than 0.02) for practical use.

TABLE 11. VOLATILE ANALYTES NOT DETECTED IN GC/MS ANALYSIS AND RECOMMENDATIONS FOR FURTHER WORK

NO.	SUBSTANCE	LIST(a)	CAS NO.	RCRA NUMBER	RECOMMENDATION FOR FURTHER WORK
1	BIS(CHLOROMETHYL) ETHER	8	542-88-1		None; Unstable
2	2-BUTANONE PEROXIDE	8	1338-23-4	U160	None; unstable
3	CHLOROMETHYL METHYL ETHER	8	107-30-2	U046	None; unstable
4	1,1-DIMETHYLHYDRAZINE	8	57-14-7	U098	Test as semivolatile or ion chromatography
5	1,2-DIMETHYLHYDRAZINE	8	540-73-8	U099	Test as semivolatile or ion chromatography
6	ETHYLENIMINE	8	151-56-4	P054	Test as semivolatile or ion chromatography
7	HEXACHLOROPROPENE	8	1888-71-7	U243	Test as semivolatile
8	N-(2-HYDROXYETHYL)ETHYLENEIMINE	M	1072-52-2	U289	Ion chromatography
9	2-METHYLAZIRIDINE	8	75-55-8	P067	Test as semivolatile or ion chromatography
10	METHYLHYDRAZINE	8	60-34-4	P068	Test as semivolatile or ion chromatography
11	METHYL ISOCYANATE	8	624-83-9	P064	None; unstable in water
12	2-METHYLLACTONITRILE	8	75-86-5	P069	None; unstable in water
13	METHYL MERCAPTAN	8	74-93-1		Other GC column with sulfur detector
14	TETRANITROMETHANE	8	509-14-8	P112	Test as semivolatile
15	THIOPHENOL	8	108-98-5	P104	Test as semivolatile

(a) 8 = Appendix VIII; M = Michigan list

TABLE 12. SEMIVOLATILE ANALYTES TESTED FOR GC-MS SUITABILITY

NO.	SUBSTANCE	LIST(a)		CAS NO.	RCRA NUMBER	STATUS CODE(b)
1	ACETOPHENONE	8		98-86-2	U004	S
2	2-ACETYLAMINOFLUORENE	8		53-96-3	U005	S
3	1-ACETYL-2-THIOUREA	8		591-08-2	P002	LR
4	ACRYLAMIDE	8		79-06-1		ND
5	ALDICARB	8		116-06-3		ND
6	2-AMINOANTHRAQUINONE		M	117-79-3	U264	S
7	AMINOAZOBENZENE		M	60-09-3	U257	S
8	4-AMINOBIPHENYL	8	M	92-67-1	U274	S
9	3-AMINO-9-ETHYLCARBAZOLE		M	132-32-1	U253	ES
10	AMITROLE	8		61-82-5	U011	ND
11	ANILAZINE		M	101-05-3	U333	S
12	ANILINE	8		62-53-3		ES
13	o-ANISIDINE		M	90-04-0	U260	S
14	ARAMITE	8	M	140-57-8	U326	S
15	AURAMINE	8		492-80-8	U014	ND
16	AZINPHOS-METHYL		M	86-50-0	P151	S
17	BARBAN		M	101-27-9	U280	LR
18	BENOMYL		M	17804-35-2	U271	ND
19	p-BENZOQUINONE	8		106-51-4	U197	S
20	BROMOXYNIL		M	1689-84-5	U272	S
21	BRUCINE	8		357-57-3	P018	ND
22	CAPTAFOL		M	2425-06-1	U285	S
23	CAPTAN		M	133-06-2	U266	S
24	CARBARYL		M	63-25-2	U279	S
25	CARBOFURAN		M	1563-66-2	U127	S
26	CARBOPHENOTHION		M	786-19-6	U148	S
27	CHLORFENVINPHOS		M	470-90-6	P143	S
28	4-CHLOROANILINE	8		106-47-8		S
29	CHLOROBENZILATE	8		510-15-6	U038	S
30	5-CHLORO-2-METHYLANILINE		M	95-79-4	U329	S
31	3-(CHLOROMETHYL)PYRIDINE HYDROCHLORIDE		M	6959-48-4	U319	S
32	4-CHLORO-1,3-PHENYLENEDIAMINE		M	5131-60-2	U305	ES
33	4-CHLORO-1,2-PHENYLENEDIAMINE		M	95-83-0	U306	ES
34	COUMAPHOS		M	56-72-4	P130	S
35	p-CRESIDINE		M	120-71-8	U262	S
36	CROTOXYPHOS		M	7700-17-6	U238	S
37	CUPFERRON		M	135-20-6	U290	ND
38	CYCLOHEXIMIDE		M	66-81-9	P134	ND
39	2-CYCLOHEXYL-4,6-DINITROPHENOL	8		131-89-5	P034	LR
40	CYCLOPHOSPHAMIDE	8		50-18-0	U058	ND
41	DEMETON		M	8065-48-3	P155	S
42	DIALLATE	8		2303-16-4	U062	S
43	2,4-DIAMINOANISOLE SULFATE		M	39156-41-7	U307	ND
44	2,4-DIAMINOTOLUENE	8	M	95-80-7	U327	S
45	DIAZINON		M	333-41-5	U313	ES
46	1,2:7,8-DIBENZACRIDINE	8		224-42-0		S
47	1,2:4,5-DIBENZOPYRENE	8		192-65-4		S
48	DICHLONE		M	117-80-6	U299	S

TABLE 12. (Continued)

NO.	SUBSTANCE	LIST(a)	CAS NO.	RCRA NUMBER	STATUS CODE(b)
49	2,6-DICHLOROPHENOL	8	87-65-0		S
50	DICHLOROVOS	M	62-73-7	P144	S
51	DICROTOPHOS	M	141-66-2	P146	S
52	DIETHYLSTILBESTROL	8	56-53-1	U086	S
53	DIETHYL SULFATE	M	64-67-5	U325	LR
54	DIHYDROSAFROLE	8	56312-13-1	U090	ND
55	DIMETHOATE	8	60-51-5		S
56	3,3'-DIMETHOXYBENZIDINE	8	119-90-4	U091	LR
57	1,4-DIMETHYLAMINOAZOBENZENE	8	60-11-7	U093	S
58	7,12-DIMETHYLBENZ(A)ANTHRACENE	8	57-97-6	U094	S
59	3,3'-DIMETHYLBENZIDINE	8	119-93-7	U095	S
60	1,1-DIMETHYLHYDRAZINE	8	57-14-7	U098	ND
61	1,2-DIMETHYLHYDRAZINE	8	540-73-8	U099	ND
62	a,a-DIMETHYLPHENETHYLAMINE	8	122-09-8	P046	S
63	1,2-DINITROBENZENE	8	99-65-0		S
64	1,3-DINITROBENZENE	8	528-29-0		S
65	1,4-DINITROBENZENE	8	100-25-4		S
66	DINOCAP	M	39300-45-3	U284	S
67	DINOSEB	8	88-85-7		S
68	DIOXATHION	M	78-34-2	P153	S
69	5,5-DIPHENYLHYDANTOIN	M	57-41-0		S
70	1,2-DIPHENYLHYDRAZINE	8	122-66-7	U109	ND
71	DISULFOTON	8	298-04-4		S
72	DPN	M	2104-64-5	P141	S
73	DITHION	M	563-12-2	P154	S
74	ETHYL CARBAMATE	8	51-79-6	U238	S
75	ETHYLENIMINE	8	151-56-4	P054	ND
76	ETHYLENE THIOUREA	8	96-45-7		ND
77	ETHYL METHANESULFONATE	8	62-50-0	U119	S
78	FAMPHUR	8	52-85-7	P097	S
79	FENSULFOTHION	M	115-90-2	P156	S
80	FENTHION	M	55-38-9		S
81	FLUCHLORALIN	M	33245-39-5	U330	S
82	2-FLUOROACETAMIDE	8	640-19-7	P057	ND
83	HEXACHLOROPHENE	8	70-30-4	U132	S
84	HEXACHLOROPROPENE	8	1888-71-7	U243	S
85	HEXAMETHYL PHOSPHORAMIDE	M	680-31-9	U312	S
86	HYDROQUINONE	M	123-31-9		S
87	ISODRIN	8	465-73-6	P060	S
88	ISONICOTINIC ACID HYDRAZIDE	M	54-85-3		ND
89	ISOSAFROLE	8	120-58-1	U141	S
90	KEPONE	8	143-50-0		S
91	LEPTOPHOS	M	21609-90-5	P140	S
92	MALATHION	M	121-75-5	U324	S
93	MALEIC ANHYDRIDE	8	108-31-6	U147	S
94	MALEIC HYDRAZIDE	8	123-33-1		ND
95	MESTRANOL	M	72-33-3	U301	S
96	METHAPYRILENE	8	91-80-5	U155	S

TABLE 12. (Continued)

NO.	SUBSTANCE	LIST(a)		CAS NO.	RCRA NUMBER	STATUS CODE(b)
97	METHOMYL	8		16752-77-5	P066	ND
98	p,p'-METHOXYCHLOR	8		72-43-5		S
99	2-METHYLAZIRIDINE	8		75-55-8	P067	ND
100	3-METHYLCHOLANTHRENE	8		56-49-5	U157	S
101	4,4'-METHYLENEBIS(2-CHLOROANILINE)	8		101-14-4	U158	LR
102	4,4'-METHYLENEBIS(N,N-DIMETHYL-ANILINE)		M	101-61-1	U255	ES
103	METHYLHYDRAZINE	8		60-34-4	P068	ND
104	METHYL METHANESULFONATE	8				S
105	N-METHYL-N-NITRO-N-NITROSOGUANIDINE	8		70-25-7	U163	ND
106	METHYL PARATHION	8		298-00-0		S
107	2-METHYLPHENOL	8		95-48-7		S
108	3-METHYLPHENOL	8		108-39-4		S
109	4-METHYLPHENOL	8		106-44-5		S
110	METHYLTHIOURACIL	8		56-04-2	U164	ND
111	MEVINPHOS		M	7786-34-7	P131	S
112	MEXACARBATE		M	315-18-4	P128	S
113	MIREX		M	2385-85-5	U297	S
114	MONOCROTOPHOS		M	6923-22-4	P147	S
115	NALED		M	300-76-5	U309	S
116	1,5-NAPHTHALENEDIAMINE		M	2243-62-1	U298	ND
117	1,4-NAPHTHOQUINONE	8		130-15-4	U166	S
118	1-NAPHTHYLAMINE	8		134-32-7	U167	S
119	2-NAPHTHYLAMINE	8		91-59-8	U168	ES
120	1-NAPHTHYL-2-THIOUREA	8		86-88-4	P072	ND
121	NICLOSAMIDE		M	50-65-7	U321	ND
122	NICOTINE	8		54-11-5	P075	S
123	5-NITROACENAPHTHENE		M	602-87-9	U250	S
124	4-NITROANILINE	8		100-01-6		S
125	5-NITRO-o-ANISIDINE		M	99-59-2	U263	S
126	4-NITROBIPHENYL		M	92-93-3	U275	S
127	NITROFEN		M	1836-75-5	U288	S
128	NITROGEN MUSTARD	8	M	51-75-2	P132	ND
129	NITROGLYCERINE	8		55-63-0	P081	ND
130	5-NITRO-O-TOLUIDINE	8		99-55-8	U181	S
131	4-NITROQUINOLINE-1-OXIDE	8		56-57-5		S
132	N-NITROSODIBUTYLAMINE	8		924-16-3		S
133	N-NITROSODIETHANOLAMINE	8		1116-54-7	U173	ND
134	N-NITROSODIETHYLAMINE	8		55-18-5		S
135	p-NITROSODIPHENYLAMINE		M	156-10-5	U287	ES
136	N-NITROSO-N-ETHYLUREA	8		759-73-9	U176	ND
137	N-NITROSOMETHYLETHYLAMINE	8		10595-95-6		S
138	N-NITROSO-N-METHYLUREA	8		684-93-5	U177	ND
139	N-NITROSO-N-METHYLURETHANE	8		615-53-2	U178	ND
140	N-NITROSOMORPHOLINE	8		59-89-2		ES
141	N-NITROSOPIPERIDINE	8		100-75-4	U176	S
142	N-NITROSOPYRROLIDINE	8		930-55-2		S
143	OCTAMETHYL PYROPHOSPHORAMIDE	8		152-16-9	P085	LR
144	OXYDEMETON-METHYL		M	301-12-2	P157	ND

TABLE 12. (Continued)

NO.	SUBSTANCE	LIST(a)		CAS NO.	RCRA NUMBER	STATUS CODE(b)
145	4,4'-OXYDIANILINE		M	101-80-4	U303	S
146	PARATHION ETHYL	8		56-38-2		S
147	PENTACHLOROBENZENE	8		608-93-5		S
148	PENTACHLORONITROBENZENE	8		82-68-8		S
149	PHENACETIN	8		62-44-2	U187	S
150	PHENAZOPYRIDINE HYDROCHLORIDE		M	136-40-3	U320	ND
151	PHENOBARBITAL		M	50-06-6	U268	S
152	1,2-PHENYLENEDIAMINE	8		95-54-5		ND
153	1,3-PHENYLENEDIAMINE	8		108-45-2		ND
154	1,4-PHENYLENEDIAMINE	8		106-50-3		S
155	N-PHENYLTHIOUREA	8		103-85-5	P093	ND
156	PHORATE	8		298-02-2		S
157	PHOSALONE	8		2310-17-0		S
158	PHOSMET		M	732-11-6		S
159	PHOSPHAMIDON		M	13171-21-6	P145	S
160	PHTHALIC ANHYDRIDE	8		85-44-9	U190	S
161	PIPERONYL SULFOXIDE		M	120-62-7	U270	S
162	PRONAMIDE	8		23950-58-5		S
163	1,3-PROPANE SULTONE	8		1120-71-4	U193	ND
164	PROPYLTHIOURACIL	8	M	51-52-5	U334	LR
165	RESORCINOL	8		108-46-3		S
166	ROTENONE		M	83-79-4	U273	ND
167	SACCHARIN	8		81-07-2	U202	ND
168	SAFROLE	8		94-59-7	U203	S
169	STRYCHNINE	8		57-24-9		S
170	SULFALLATE		M	95-06-7	U277	S
171	TERBUFOS		M	13071-79-9	P149	S
172	1,2,4,5-TETRACHLOROBENZENE	8		95-94-3		S
173	2,3,4,6-TETRACHLOROPHENOL	8		58-90-2		S
174	TETRACHLORVINPHOS		M	961-11-5	U308	S
175	TETRAETHYL DITHIOPYROPHOSPHATE	8		3689-24-5	P109	ES
176	TETRAETHYL PYROPHOSPHATE	8		107-49-3		S
177	TETRANITROMETHANE	8		509-14-8	P112	ND
178	THIOACETAMIDE	8		62-55-5	U128	S
179	THIOFANOX	8		39196-18-4	P045	ND
180	THIONAZINE	8		297-97-2	P040	S
181	THIOPHENOL	8		108-98-5	P104	S
182	TOLUENE DIISOCYANATE	8		584-84-9	U223	S
183	o-TOLUIDINE	8	M	95-53-4	U328	S
184	TRICHLORFON		M	52-68-6	P139	ND
185	2,4,5-TRICHLOROPHENOL	8		95-95-4		S
186	O,O,O-TRIETHYL PHOSPHOROTHIOATE	8		126-68-1		ES
187	TRIFLURALIN		M	1582-09-8	U332	S
188	2,4,5-TRIMETHYLANILINE		M	137-17-7	U259	S
189	TRIMETHYL PHOSPHATE		M	512-56-1	U310	S
190	1,3,5-TRINITROBENZENE	8		99-35-4	U234	S
191	TRIS(2,3-DIBROMOPROPYL) PHOSPHATE	8		126-72-7	U235	LR
192	TRI-p-TOLYL PHOSPHATE(c)		M	78-32-0		S

TABLE 12. (Continued)

NO.	SUBSTANCE	LIST(a)	CAS NO.	RCRA NUMBER	STATUS CODE(b)
193	WARFARIN	8	81-81-2	P001	ND

(a) 8 = Appendix VIII; M = Michigan list

(b) S - apparently suitable for GC-MS analysis
LR - low response; response factor, versus phenanthrene -D10, less than 0.02
ND - not detected
ES - expected to be suitable for GC/MS analysis but not detected in this study

(c) Substitute for the non-specific mixture, tricresyl phosphate

TABLE 13. GC AND MS CHARACTERISTICS FOR SEMIVOLATILE ANALYTES THAT WERE DETECTED

NO.	SUBSTANCE	LIST(a)		CAS NO.	RCRA NUMBER	MS LIB. NUMBER(b)	RT (MIN)	RRI(d)	RECOMMENDED QUAN ION	RECOMMENDED SEARCH IONS IN DECENDING ORDER OF IMPORTANCE (RELATIVE ABUNDANCE)	RESPONSE FACTOR(e)
1	ACETOPHENONE	8		98-86-2	U004	3031	12.67	0.416	105	77 (100) 105 (95) 51 (40) 120 (25)	0.368
2	2-ACETYLAMINOFLUORENE	8		53-96-3	U005	19378	33.58	1.104	181	181 (100) 180 (90) 223 (65) 152 (45)	0.111
3	1-ACETYL-2-THIOUREA	8		591-08-2	P002	2799	18.22	0.599	118	43 (100) 118 (15) 42 (25) 76 (5)	0.002 (c)
4	2-AMINOANTHRAQUINONE		M	117-79-3	U264	19369	30.63	1.411	223	223 (100) 167 (40) 195 (35)	0.139
5	AMINOAZOBENZENE		M	60-09-3	U257	15498	25.72	1.184	197	92 (100) 197 (40) 120 (35) 65 (40) 77 (25)	0.230
6	4-AMINOBIPHENYL	8	M	92-67-1	U274	10938	25.08	0.824	169	169 (100) 168 (25) 170 (15) 115 (15)	0.087
7	ANILAZINE		M	101-05-3	U333	25458	28.47	1.149	239	239 (100) 241 (60) 143 (55) 178 (45) 89 (25)	0.021
8	o-ANISIDINE		M	90-04-0	U260	3249	15.00	0.493	108	80 (100) 108 (95) 123 (55) 52 (35)	0.226
9	ARAMITE	8	M	140-57-8	U326	30755	30.92	1.016	185	185 (100) 191 (50) 319 (55) 334 (35) 197 (30) 321 (20)	0.091
10	AZINPHOS-METHYL		M	86-50-0	P151	29421	35.25	1.158	160	160 (100) 132 (75) 93 (60) 104 (35) 105 (25)	0.022
11	BARBAN		M	101-27-9	U280	23539	30.83	1.013	222	222 (100) 51 (95) 87 (55) 224 (35) 257 (25) 153 (40)	0.015 (c)
12	p-BENZOQUINONE	8		106-51-4	U197	1743	9.13	0.300	108	54 (100) 108 (75) 82 (40) 80 (30)	0.171
13	BROMOXYNIL		M	1689-84-5	U272	25508	23.90	0.785	277	277 (100) 279 (50) 88 (45) 275 (53) 168 (15)	0.181
14	CAPTAFOL		M	2425-06-1	U285	31611	33.47	1.100	79	79 (100) 77 (30) 80 (25) 107 (10)	0.095
15	CAPTAN		M	133-06-2	U266	27860	29.47	0.968	79	79 (100) 149 (25) 77 (35) 119 (19) 117 (17)	0.048
16	CARBARYL		M	63-25-2	U279	16133	27.17	0.893	144	144 (100) 115 (55) 116 (30) 201 (5)	0.380
17	CARBOFURAN		M	1563-66-2	U127	19005	24.90	0.818	164	164 (100) 149 (65) 131 (20) 122 (17)	0.232
18	CARBOPHENOTHION		M	786-19-6	U148		28.58	1.318	157	157 (100) 97 (55) 121 (45) 342 (25) 159 (35) 199 (25)	0.273
19	CHLORFENVINPHOS		M	470-90-6	P143	32264	29.53	0.971	267	267 (100) 269 (65) 323 (65) 325 (45) 295 (20)	0.120
20	4-CHLOROANILINE	8		106-47-8		3740	15.50	0.509	127	127 (100) 129 (35) 65 (45) 92 (15)	0.108
21	CHLOROBENZILATE	8		510-15-6	U038	29969	31.77	1.044	251	251 (95) 139 (100)253 (65) 111 (50) 141 (35)	0.357
22	5-CHLORO-2-METHYLANILINE		M	95-79-4	U329	5890	14.28	0.658	106	106 (100) 141 (95) 140 (75) 77 (70) 89 (30)	0.195
23	3-(CHLOROMETHYL)PYRIDINE HYDROCHLORIDE		M	6959-48-4	U319		17.50	0.543	92	92 (100) 127 (45) 129 (15) 65 (50) 39 (35)	(f)
24	COUMAPHOS		M	56-72-4	P130	32529	37.08	1.219	362	362 (100) 226 (45) 210 (30) 364 (40) 97 (35) 109 (30)	0.064
25	p-CRESIDINE		M	120-71-8	U252	5213	16.45	0.664	122	122 (100) 94 (70) 137 (65) 77 (30) 93 (15)	0.225
26	CROTOXYPHOS		M	7700-17-6	U238	29095	29.73	0.977	127	127 (100) 105 (60) 193 (45) 166 (30)	0.106
27	2-CYCLOHEXYL-4,6-DINITROPHENOL	8		131-89-5	P034	24443	26.87	1.237	231	231 (50) 185 (45) 41 (100)193 (40) 266 (25)	0.019 (c)
28a	DEMETON-O		M	298-03-3	P155		22.72	0.913	88	88 (100) 89 (60) 60 (40) 61 (30) 115 (15) 171 (10)	0.539
28b	DEMETON-S		M	126-75-0	P155		24.30	0.977	88	88 (100) 60 (40) 81 (15) 89 (15) 114 (15) 115 (10)	0.775
29a	DIALLATE (CIS OR TRANS)	8		2303-16-4	U062		20.57	0.949	86	86 (55) 234 (35) 43 (100) 70 (20)	0.364
29b	DIALLATE (TRANS OR CIS)	8		2303-16-4	U062		20.78	0.959	86	86 (60) 234 (40) 43 (100) 70 (15)	0.350
30	2,4-DIAMINOTOLUENE	8	M	95-80-7	U327	3162	15.78	0.727	121	121 (100) 122 (90) 94 (25) 77 (20) 104 (15)	0.152
31	1,2:7,8-DIBENZACRIDINE	8		224-42-0			36.40	1.676	279	279 (100) 280 (25) 277 (15) 250 (5)	0.505

TABLE 13. (Continued)

NO	SUBSTANCE	LIST(a)	CAS NO.	RCRA NUMBER	MS LIB. NUMBER(b)	RT (MIN)	RRI(d)	RECOMMENDED QUAN ION	RECOMMENDED SEARCH IONS IN DECENDING ORDER OF IMPORTANCE (RELATIVE ABUNDANCE)	RESPONSE FACTOR(e)
32	1,2:4,5-DIBENZOPYRENE	8	192-65-4			41.60	19.16	302	302 (100) 151 (70) 150 (65) 300 (25)	0.455
33	DICHLONE	M	117-80-6	U299	19711	25.77	0.847	191	191 (100) 163 (85) 226 (65) 228 (45) 135 (50) 193 (35)	0.174
34	2,6-DICHLOROPHENOL	8	87-65-0		9673	15.47	0.508	162	162 (100) 164 (65) 126 (25) 98 (30) 63 (80)	0.298
35	DICHLOROVOS	M	62-73-7	P144	18944	16.48	0.542	109	109 (100) 185 (25) 79 (25) 145 (10)	0.199
36	DICROTOPHOS	M	141-66-2	P146	21176	23.82	0.783	127	127 (100) 67 (25) 72 (15) 109 (10) 193 (10) 237 (5)	0.158
37	DIETHYLSTILBESTEROL	8	56-53-1	U086		32.15	1.292	268	268 (100) 145 (90) 107 (85) 239 (65) 121 (25) 159 (25)	0.153
38	DIETHYL SULFATE	M	64-67-5	U325	8164	11.37	0.374	139	139 (35) 45 (100) 59 (75) 99 (35) 111 (45) 125 (40)	0.019 (c)
39	DIHYDROSAFFROLE	8	56312-13-1	U090		22.42	0.693	135	135 (100) 64 (25) 77 (28)	(g)
40	DIMETHOATE	8	60-51-5		20253	24.70	0.812	87	87 (100) 93 (65) 125 (50) 143 (10) 229 (5)	0.174
41	3,3'-DIMETHOXYBENZIDINE	8	119-90-4	U091	22015	34.47	1.133	244	244 (100) 201 (75) 229 (45)	0.016 (c)
42	DIMETHYLAMINOAZOBENZENE	8	60-11-7	U093	19680	27.50	1.266	225	225 (60) 120 (100) 77 (55) 105 (25) 148 (20) 42 (70)	0.244
43	7,12-DIMETHYLBENZ(A)ANTHRACENE	8	57-97-6	U094	23504	33.25	1.531	256	256 (100) 241 (65) 239 (50) 120 (50)	0.407
44	3,3'-DIMETHYLBENZIDINE	8	119-93-7	U095	17852	28.55	1.315	212	212 (100) 106 (20) 196 (12) 180 (10)	0.355
45	α,α-DIMETHYLPHENETHYLAMINE	8	122-09-8	P046	7163	25.43	0.789	58	58 (100) 91 (10) 65 (5) 134 (5) 42 (10)	0.175
46	1,2-DINITROBENZENE	8	99-65-0		10822	20.58	0.676	168	168 (50) 50 (100) 63 (85) 74 (50)	0.050
47	1,3-DINITROBENZENE	8	528-29-0			20.18	0.663	168	168 (95) 76 (100) 50 (85) 75 (95) 92 (45) 122 (40)	0.137
48	1,4-DINITROBENZENE	8	100-25-4		10823	19.83	0.652	168	168 (90) 75 (100) 50 (85) 76 (80) 92 (30) 122 (30)	0.131
49	DINOCAP	M	39300-45-3	U294	32678	33.47	1.100	69	69 (100) 41 (30) 39 (15)	0.047
50	DINOSEB	8	88-85-7		21460	25.83	0.849	211	211 (100) 163 (50) 147 (35) 117 (30) 240 (15)	0.137
51	DIOXATHION	M	78-34-2	P153	36614	25.25	0.830	97	97 (100) 125 (55) 270 (40) 153 (20)	0.047
52	5,5-DIPHENYLHYDANTOIN	M	57-41-0		22930	33.40	1.098	180	180 (100) 104 (50) 252 (45) 223 (50) 209 (40)	0.073
53	DISULFOTON	8	298-04-4		25449	25.83	0.849	88	88 (100) 97 (35) 89 (40) 142 (20) 186 (10)	0.385
54	EPN	M	2104-64-5	P141	29898	30.11	1.389	157	157 (100) 169 (55) 185 (30) 141 (30) 323 (10)	0.321
55	ETHION	M	563-12-2	P154	33771	32.08	1.054	231	231 (70) 97 (100)153 (65) 125 (55) 121 (40)	0.215
56	ETHYL CARBAMATE	8	51-79-6	U238	746	7.27	0.239	62	62 (90) 44 (100) 45 (70) 74 (15)	0.055
57	ETHYL METHANESULFONATE	8	62-50-0	U119	3289	9.62	0.316	79	79 (100) 109 (45) 97 (20) 45 (20) 65 (15)	0.139
58	FAMPHUR	8	52-85-7	P097	30037	32.67	1.074	218	218 (100) 125 (30) 93 (30) 109 (10) 217 (25)	0.133
59	FENSULFOTHION	M	115-90-2	P156	28592	31.87	1.047	293	293 (100) 97 (70) 308 (40) 125 (50) 292 (55)	0.050
60	FENTHION	M	55-38-9		25683	28.37	0.932	278	278 (100) 125 (45) 109 (35) 169 (25) 153 (20)	0.321
61	FLUCHLORALIN	M	33245-39-5	U330	32127	25.88	0.851	306	306 (100) 63 (99) 326 (80) 328 (25) 264 (60) 65 (35)	0.122
62	HEXACHLOROPHENE	8	70-30-4	U132	34710	47.98	1.488	196	196 (100) 198 (98) 209 (60) 211 (55) 406 (12) 408 (10)	0.038
63	HEXACHLOROPROPENE	8	1888-71-7	U243	22282	12.45	0.573	213	213 (100) 211 (60) 215 (60) 117 (30) 106 (30) 141 (20)	0.211
64	HEXAMETHYL PHOSPHORAMIDE	M	680-31-9	U312	12578	17.33	0.570	135	135 (75) 44 (100)179 (35) 92 (25) 42 (45)	0.129

TABLE 13. (Continued)

NO.	SUBSTANCE	LIST(a)	CAS NO.	RCRA NUMBER	MS LIB. NUMBER(b)	RT (MIN)	RRI(d)	RECOMMENDED QUAN ION	RECOMMENDED SEARCH IONS IN DECENDING ORDER OF IMPORTANCE (RELATIVE ABUNDANCE)	RESPONSE FACTOR(e)
65	HYDROQUINONE	M	123-31-9		1900	16.93	0.556	110	110 (100) 81 (65) 53 (55) 55 (35)	0.021
66	ISODRIN	8	465-73-6	P060	32527	28.95	0.951	193	193 (80) 66 (100)195 (75) 263 (45) 265 (30) 147 (25)	0.161
67	ISOSAFROLE	8	120-58-1	U141	9490	15.60	0.719	162	162 (100) 131 (50) 104 (45) 77 (40) 51 (25)	0.527
68	KEPONE	8	143-50-0		37389	28.18	1.300	272	272 (100) 274 (80) 237 (50) 178 (35) 143 (45) 270 (55)	0.073
69	LEPTOPHOS	M	21609-90-5	P140	34913	35.28	1.159	171	171 (100) 377 (75) 375 (55) 77 (50) 155 (25) 379 (20)	0.214
70	MALATHION	M	121-75-5	U324	30376	28.08	0.923	173	173 (99) 125 (100)127 (85) 93 (90) 158 (40)	0.139
71	MALEIC ANHYDRIDE	8	108-31-6	U147	1010	7.65	0.251	54	54 (100) 98 (15) 53 (20) 44 (10)	0.134
72	MESTRANOL	M	72-33-3	U301	28817	36.48	1.199	227	227 (100) 310 (65) 174 (30) 147 (20) 242 (15)	0.145
73	METHAPYRILENE	8	91-80-5	U155	24001	28.77	0.945	97	97 (50) 50 (100)191 (10) 71 (15)	0.022
74	METHOXYCHLOR	8	72-43-5		31412	33.55	1.349	227	227 (100) 228 (20) 152 (10) 114 (10) 274 (5) 212 (5)	0.466
75	3-METHYLCHOLANTHRENE	8	56-49-5	U157	24784	35.07	1.615	268	268 (100) 252 (50) 253 (45) 126 (45) 134 (20) 113 (15)	0.377
76	4,4'-METHYLENEBIS(2-CHLOROANILINE)	8	101-14-4	U158	24450	34.38	1.130	231	231 (100) 266 (70) 268 (45) 140 (45) 195 (35)	0.010 (c)
77	METHYLMETHANESULFONATE	8				7.48	0.301	80	80 (100) 79 (85) 65 (25) 95 (20)	0.396
78	METHYL PARATHION	8	298-00-0		24219	27.03	0.888	109	109 (100) 125 (80) 263 (60) 79 (35) 93 (20)	0.258
79	2-METHYLPHENOL	8	95-48-7		1771	12.40	0.407	107	107 (100) 108 (95) 77 (65) 79 (55) 90 (30)	0.203
80	3-METHYLPHENOL	8	108-39-4		1775	12.93	0.425	107	107 (100) 108 (85) 77 (45) 79 (45) 90 (15)	0.264
81	4-METHYLPHENOL	8	106-44-5		1774	12.82	0.421	107	107 (100) 108 (75) 77 (35) 79 (25) 90 (10)	0.416
82	MEVINPHOS	M	7786-34-7	P131	19593	19.90	0.654	127	127 (100) 192 (25) 109 (30) 67 (20) 164 (10)	0.164
83	MEXACARBATE	M	315-18-4	P128	19119	26.02	0.855	165	165 (100) 150 (35) 134 (20) 164 (35) 222 (10)	0.124
84	MIREX	M	2385-85-5	U297	38190	35.43	1.164	272	272 (100) 237 (25) 274 (35) 270 (25) 239 (15) 235 (15)	0.216
85	MONOCROTOPHOS	M	6923-22-4	P147	19197	24.08	0.791	127	127 (100) 192 (5) 67 (10) 97 (10) 109 (5)	0.168
86	NALED	M	300-76-5	U309	33491	20.03	0.924	109	109 (100) 145 (50) 147 (15) 301 (15) 79 (15) 189 (10)	0.155
87	1,4-NAPHTHOQUINONE	8	130-15-4	U166	8839	16.23	0.747	158	158 (100) 104 (55) 102 (50) 76 (50) 50 (40) 130 (35)	0.322
88	1-NAPHTHYLAMINE	8	134-32-7	U167	6207	18.20	0.838	143	143 (100) 115 (50) 89 (10) 63 (10)	0.668
89	NICOTINE	8	54-11-5	P075	9534	18.70	0.615	84	84 (100) 133 (20) 161 (10) 162 (10)	0.178
90	5-NITROACENAPHTHENE	M	602-87-9	U250		28.73	0.944	199	199 (35) 152 (100)169 (15) 141 (15) 115 (10)	0.225
91	4-NITROANILINE	8	100-01-6		5358	19.37	0.892	138	138 (85) 65 (100)108 (40) 92 (35) 80 (20) 39 (45)	0.150
92	5-NITRO-o-ANISIDINE	M	99-59-2	U263	10836	21.50	0.990	168	168 (100) 79 (90) 52 (85) 138 (65) 153 (50) 77 (40)	0.199
93	4-NITROBIPHENYL	M	92-93-3	U275	15854	26.55	0.872	199	199 (95) 152 (100)141 (30) 169 35) 151 (30)	0.202
94	NITROFEN	M	1836-75-5	U288	26234	31.48	1.035	283	283 (100) 285 (65) 202 (45) 139 (25) 253 (15)	0.121
95	5-NITRO-o-TOLUIDINE	8	99-55-8	U181	7752	19.27	0.887	152	77 (100) 152 (90) 79 (55) 106 (55) 94 (20)	0.276
96	4-NITROQUINOLINE-1-OXIDE	8	56-57-5			21.73	0.714	174	174 (65) 101 (100)128 (95) 75 (70) 116 (65)	0.042
97	N-NITROSODIBUTYLAMINE	8	924-16-3		8954	16.73	0.550	84	84 (100) 57 (70) 41 (80) 116 (20) 158 (10)	0.177

TABLE 13. (Continued)

NO.	SUBSTANCE	LIST(a)	CAS NO.	RCRA NUMBER	MS LIB. NUMBER(b)	RT (MIN)	RRI(d)	RECOMMENDED QUAN ION	RECOMMENDED SEARCH IONS IN DECENDING ORDER OF IMPORTANCE (RELATIVE ABUNDANCE)	RESPONSE FACTOR(e)
98	N-NITROSODIETHYLAMINE	8	55-18-5		1410	8.70	0.286	102	102 (60) 42 (100) 57 (40) 44 (55) 56 (40)	0.098
99	N-NITROSOMETHYLETHYLAMINE	8	10595-95-6			6.97	0.229	88	42 (100) 88 (55) 43 (60) 56 (20)	0.062
100	N-NITROSOPIPERIDINE	8	100-75-4	U176	2332	13.55	0.445	114	42 (100) 114 (50) 55 (55) 56 (30) 41 (35)	0.070
101	N-NITROSOPYRROLIDINE	8	930-55-2		1215	12.65	0.416	100	100 (60) 41 (100) 42 (55) 68 (25) 69 (25)	0.057
102	OCTAMETHYL PYROPHOSPHORAMIDE	8	152-16-9	P085	26664	24.93	0.819	135	135 (65) 44 (100)199 (45) 286 (35) 153 (35) 243 (25)	0.014 (c)
103	4,4'-OXYDIANILINE	M	101-80-4	U303	15962	26.08	1.201	200	200 (100) 108 (55) 171 (30) 80 (30) 65 (30)	0.125
104	PARATHION ETHYL	8	56-38-2		27067	28.40	0.933	109	109 (100) 97 (95) 291 (50) 139 (50) 155 (35)	0.187
105	PENTACHLOROBENZENE	8	608-93-5		22534	21.35	0.702	250	250 (100) 252 (65) 108 (45) 248 (60) 215 (25) 254 (20)	0.263
106	PENTACHLORONITROBENZENE	8	82-68-8		27251	21.72	1.001	237	237 (100) 142 (90) 214 (80) 249 (75) 295 (55) 265 (30)	0.080
107	PHENACETIN	8	62-44-2	U187	12523	24.33	0.800	108	180 (100) 179 (70) 109 (75) 137 (40) 80 (30)	0.136
108	PHENOBARBITAL	M	50-06-6	U268	20538	24.70	1.137	204	204 (100) 117 (35) 232 (20) 146 (15) 161 (15)	0.331
109	1,4-PHENYLENEDIAMINE	8	106-50-3		1746	13.62	0.627	108	108 (100) 80 (50) 53 (25) 54 (23) 52 (15)	0.239
110	PHORATE	8	298-02-2		23956	24.10	0.792	75	75 (100) 121 (30) 97 (25) 93 (15) 260 (10)	0.294
111	PHOSALONE	8	2310-17-0			35.23	1.158	182	182 (100) 184 (30) 367 (35) 121 (30) 379 (15)	0.062
112	PHOSMET	M	732-11-6		29423	30.03	1.385	160	160 (100) 77 (10) 93 (10) 317 (5) 76 (5)	0.631
113	PHOSPHAMIDON	M	13171-21-6	P145	27796	26.85	0.882	127	127 (100) 264 (40) 72 (50) 109 (50) 138 (25)	0.063
114	PHTHALIC ANHYDRIDE	8	85-44-9	U190	7118	14.62	0.673	104	104 (100) 76 (90) 50 (70) 148 (35)	0.214
115	PIPERONYL SULFOXIDE	M	120-62-7	U270	29987	46.43	1.440	162	162 (100) 135 (12) 105 (8) 77 (5)	0.024
116	PRONAMIDE	8	23950-58-5		23303	25.48	0.837	173	173 (100) 175 (65) 145 (35) 109 (20) 147 (25)	0.381
117	PROPYLTHIOURACIL	8 M	51-52-5	U334	11178	27.68	0.910	170	170 (100) 142 (65) 114 (35) 83 (25)	0.016 (c)
118	RESORCINOL	8	108-46-3		1898	17.13	0.563	110	110 (100) 81 (50) 82 (40) 53 (35) 69 (30)	0.048
119	SAFROLE	8	94-59-7	U203	9487	17.23	0.566	162	162 (100) 162 (50) 104 (55) 77 (50) 103 (45) 135 (35)	0.208
120	STRYCHNINE	8	57-24-9		30807	45.15	1.484	334	334 (100) 335 (30) 333 (15)	0.099
121	SULFALLATE	M	95-06-7	U277	19398	24.23	0.796	188	188 (100) 88 (25) 72 (25) 60 (30) 44 (30)	0.187
122	TERBUFOS	M	13071-79-9	P149	26848	25.35	0.833	231	231 (45) 57 (100) 97 (30) 153 (20) 103 (25)	0.061
123	1,2,4,5-TETRACHLOROBENZENE	8	95-94-3		18165	17.97	0.590	216	216 (100) 214 (80) 179 (25) 108 (30) 143 (20) 218 (45)	0.311
124	2,3,4,6-TETRACHLOROPHENOL	8	58-90-2		20418	21.88	0.719	232	232 (100) 131 (75) 230 (75) 166 (45) 234 (50) 168 (40)	0.172
125	TETRACHLORVINPHOS	M	961-11-5	U308	32646	30.27	0.995	329	109 (100) 329 (95) 331 (90) 79 (30) 333 (30)	0.113
126	TETRAETHYL PYROPHOSPHATE	8	107-49-3		27066	11.07	0.510	99	99 (100) 155 (70) 127 (55) 81 (55) 109 (35)	0.043
127	THIONAZINE	8	297-97-2	P040	22545	19.35	0.892	107	96 (100) 107 (75) 97 (95) 143 (45) 79 (50) 68 (50)	0.109
128	THIOPHENOL (BENZENETHIOL)	8	108-98-5	P104	1903	7.42	0.342	110	110 (100) 66 (30) 109 (25) 84 (15)	0.451
129	TOLUENE DIISOCYANATE	8	584-84-9	U223	11916	18.42	0.605	174	174 (100) 145 (70) 173 (30) 146 (30) 132 (20) 91 (20)	0.178
130	o-TOLUIDINE	8 M	95-53-4	U328	1709	12.87	0.423	106	106 (100) 107 (70) 77 (35) 51 (25) 79 (25)	0.176

TABLE 13. (Continued)

NO.	SUBSTANCE	LIST(a)	CAS NO.	RCRA NUMBER	MS LIB. NUMBER(b)	RT (MIN)	RRI(d)	RECOMMENDED QUAN ION	RECOMMENDED SEARCH IONS IN DECENDING ORDER OF IMPORTANCE (RELATIVE ABUNDANCE)	RESPONSE FACTOR(e)
131	2,4,5-TRICHLOROPHENOL	8	95-95-4		15448	18.47	0.607	196	196 (100) 198 (95) 97 (75) 132 (40) 99 (30)	0.212
132	TRIFLURALIN	M	1582-09-8	U332	30852	23.88	0.785	306	306 (70) 43 (100) 264 (65) 41 (60) 290 (10)	0.173
133	2,4,5-TRIMETHYLANILINE	M	137-17-7	U259		16.70	0.674	120	120 (100) 135 (75) 134 (55) 91 (20) 77 (15)	0.307
134	TRIMETHYL PHOSPHATE	M	512-56-1	U310	5619	9.53	0.313	110	110 (100) 79 (50) 95 (35) 109 (40) 140 (10)	0.218
135	1,3,5-TRINITROBENZENE	8	99-35-4	U234		23.68	0.952	75	75 (100) 74 (60) 213 (25) 120 (25) 91 (15) 63 (15)	0.307
136	TRIS(2,3-DIBROMOPROPYL) PHOSPHATE	8	126-72-7	U235	39315	35.68	1.646	201	137 (100) 201 (30) 119 (75) 217 (50) 219 (52) 199 (20)	0.006 (e)
137	TRI-p-TOLYL PHOSPHATE(h)	M	78-32-0		32909	32.75	1.515	368	368 (100) 367 (60) 107 (70) 165 (45) 198 (30)	0.186

(a) 8 = Appendix VIII; M = Michigan list

(b) EPA/NIH Mass Spectral Data Base,1983 version; 39,763 mass spectra

(c) Response factor judged to be too low (i.e., less than 0.02) for practical use.

(d) Relative Retention Index versus phenanthrene-D10

(e)
$$\text{Response Factor} = \frac{(\text{Area quant ion}) \times (\text{Amount phenanthrene-D10})}{(\text{Area m/z = 188 for phen-D10}) \times (\text{Amount analyte})}$$

(f) Unknown concentration of stock free base prevents computation of RF

(g) Response factor not available due to partial decomposition of analyte on injection

(h) Substitute for the non-specific mixture, tricresyl phosphate

TABLE 14. SEMIVOLATILE ANALYTES EXPECTED TO BE SUITABLE FOR GC-MS ANALYSIS BUT NOT DETECTED IN THIS STUDY

NO.	SUBSTANCE	LIST(a)	CAS NO.	RCRA NUMBER
1	3-AMINO-9-ETHYLCARBAZOLE	M	132-32-1	U253
2	ANILINE	8	62-53-3	
3	4-CHLORO-1,3-PHENYLENEDIAMINE	M	5131-60-2	U305
4	4-CHLORO-1,2-PHENYLENEDIAMINE	M	95-83-0	U306
5	DIAZINON	M	333-41-5	U313
6	4,4'-METHYLENEBIS(N,N-DIMETHYLANILINE)	M	101-61-1	U255
7	2-NAPHTHYLAMINE	8	91-59-8	U168
8	p-NITROSODIPHENYLAMINE	M	156-10-5	U287
9	N-NITROSOMORPHOLINE	8	59-89-2	
10	TETRAETHYL DITHIOPYROPHOSPHATE	8	3689-24-5	P109
11	O,O,O-TRIETHYL PHOSPHOROTHIOATE	8	126-68-1	

(a) 8 = Appendix VIII; M = Michigan list

TABLE 15. SEMIVOLATILE ANALYTES NOT DETECTED AND RECOMMENDATIONS FOR FURTHER WORK

NO.	SUBSTANCE	LIST(a)		CAS NO.	RCRA NUMBER	PREDICTED CAUSE OF NON-DETECTION AND RECOMMENDATION FOR FURTHER METHOD DEVELOPMENT
1	ACRYLAMIDE(b)	8		79-06-1		Polar; polar GC column(d)
2	ALDICARB	8		116-06-3		Thermolabile; polar; HPLC-PCD(c)
3	AMITROLE	8		61-82-5	U011	Polar; HPLC
4	AURAMINE	8		492-80-8	U014	Polar; HPLC
5	BENOMYL		M	17804-35-2	U271	Thermolabile; Polar; HPLC
6	BRUCINE	8		357-57-3	P018	Basic; low volatility; HPLC; special GC conditions(e)
7	CUPFERRON		M	135-20-6	U290	Thermolabile(h); HPLC
8	CYCLOHEXIMIDE		M	66-81-9	P134	Further GC dev.(d); HPLC; or special GC(i)
9	CYCLOPHOSPHAMIDE	8		50-18-0	U058	Thermolabile; HPLC
10	2,4-DIAMINOANISOLE SULFATE		M	39156-41-7	U307	Basic, polar; HPLC or special GC(e)
11	1,1-DIMETHYLHYDRAZINE	8		57-14-7	U098	Basic, polar; ion chromatography; deriv. HPLC
12	1,2-DIMETHYLHYDRAZINE	8		540-73-8	U099	Basic, polar; ion chromatography; deriv. HPLC
13	1,2-DIPHENYLHYDRAZINE	8		122-66-7	U109	Thermolabile; HPLC
14	ETHYLENE THIOUREA	8		96-45-7		Special GC conditions(f)
15	ETHYLENIMINE	8		151-56-4	P054	Basic, polar; ion chromatography
16	2-FLUOROACETAMIDE	8		640-19-7	P057	Further GC dev.(d)
17	ISONICOTINIC ACID HYDRAZIDE		M	54-85-3		Thermolabile, polar; HPLC
18	MALEIC HYDRAZIDE	8		123-33-1		Polar, HPLC
19	METHOMYL	8		16752-77-5	P066	Thermolabile, polar; HPLC-PCD(c)
20	2-METHYLAZIRIDINE	8		75-55-8	P067	Basic, polar; ion chromatography; deriv. HPLC
21	METHYLHYDRAZINE	8		60-34-4	P068	Basic, polar; ion chromatography; deriv. HPLC
22	N-METHYL-N-NITRO-N-NITROSOGUANIDINE	8		70-25-7	U163	Thermolabile polar; HPLC
23	METHYLTHIOURACIL	8		56-04-2	U164	Thermolabile polar; HPLC
24	1,5-NAPHTHALENDIAMINE		M	2243-62-1	U298	Basic, polar; HPLC or special GC(e)
25	1-NAPHTHYL-2-THIOUREA	8		86-88-4	P072	Thermolabile polar; HPLC
26	NICLOSAMIDE		M	50-65-7	U321	Further GC dev.(d)
27	NITROGEN MUSTARD	8	M	51-75-2	P132	Thermo, hydrolabile; no recommendation
28	NITROGLYCERINE	8		55-63-0	P081	Thermolabile polar; HPLC
29	N-NITROSODIETHANOLAMINE	8		1116-54-7	P173	Thermolabile polar; HPLC
30	N-NITROSO-N-ETHYLUREA	8		759-73-9	U176	Thermolabile polar; HPLC
31	N-NITROSO-N-METHYLUREA	8		684-93-5	U177	Thermolabile polar; HPLC
32	N-NITROSO-N-METHYLURETHANE	8		615-53-2	U178	Thermolabile polar; labile; HPLC
33	OXYDEMETON-METHYL		M	301-12-2	P157	Further GC dev.(d)
34	1,2-PHENYLENEDIAMINE	8		95-54-5		Basic, polar; HPLC or special GC(e)
35	1,3-PHENYLENEDIAMINE	8		108-45-2		Basic, polar; HPLC or special GC(e)
36	N-PHENYLTHIOUREA	8		103-85-5	P093	Thermolabile polar; HPLC
37	1,3-PROPANE SULTONE	8		1120-71-4	U193	Reactive; no recommendation
38	PHENAZOPYRIDINE HYDROCHLORIDE		M	136-40-3	U320	Basic, polar; HPLC
39	ROTENONE		M	83-79-4	U273	Polar thermolabile; HPLC
40	SACCHARIN	8		81-07-2	U202	Non-volatile; Polar; HPLC

TABLE 15. (Continued)

NO.	SUBSTANCE	LIST(a)	CAS NO.	RCRA NUMBER	PREDICTED CAUSE OF NON-DETECTION AND RECOMMENDATION FOR FURTHER METHOD DEVELOPMENT
41	TETRANITROMETHANE	8	108-98-5	P104	Thermolabile; HPLC
42	THIOACETAMIDE(b)	8	62-55-5	U128	Polar; polar GC column(d)
43	THIOFANOX	8	39196-18-4	P045	Thermolabile; HPLC-PCD(c)
44	TRICHLORFON	M	52-68-6	P139	Thermolabile; special GC
45	WARFARIN	8	81-81-2	P001	Non-volatile; HPLC

(a) 8 = Appendix VIII; M = Michigan list

(b) Detected in the GC-MS data but with such poor chromatography that other GC conditions would be required for successful analysis

(c) HPLC with post-column derivitization (PCD) can be expected to be or has been shown in other research programs to be effective for this analyte

(d) There is no obvious reason why this analyte could not be analyzed by fused silica capillary GC, and it is judged likely that a GC method could be developed

(e) GC using columns which have been demonstrated to work well with amines should prove suitable so long as acidic analytes or injection conditions are avoided and the GC performance toward basic analytes is carefully monitored

(f) Specialized GC conditions using a short, polar fused silica capillary column, 250 C injector and an extremely short (10 sec) splitless time have been successfully used for this analyte.

(g) Prior research on trichlorfon has shown that it is extremely sensitive to injection decomposition but can be analyzed by GC with 150 C injector temperature or cold, on-column injection.

(h) Detection of the thermal decomposition product nitrosobenzene indicated probable quantitative decomposition of cupferon in the GC injector

(i) Has been successfully determined in aqueous media by analysis of dimethyl cyclohexanone product from caustic hydrolysis. US EPA Contract 68-03-2856.